

**Discrete-to-continuum limit for
nonlinear reaction-diffusion systems via
EDP convergence for gradient systems**

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Abstract

We investigate the convergence of spatial discretizations for reaction-diffusion systems with mass-action law satisfying a detailed balance condition. Considering systems on the d -dimensional torus, we construct appropriate space-discrete processes and show convergence not only on the level of solutions, but also on the level of the gradient systems governing the evolutions. As an important step, we prove chain rule inequalities for the reaction-diffusion systems as well as their discretizations, featuring a non-convex dissipation functional. The convergence is then obtained with variational methods by building on the recently introduced notion of gradient systems in continuity equation format.

1 Introduction

The aim of this work is to show convergence of spatial discretizations of a class of reaction-diffusion systems satisfying mass-action law. Considering finitely many species X_i with $i \in I = \{1, \dots, i_*\}$ undergoing finitely many reactions chemical reactions labeled by $r \in R := \{1, \dots, r_*\}$ and diffusing in a medium, the reaction-diffusion systems we are considering can in general be written as

$$\partial_t \rho_i = \operatorname{div}(\delta_i \rho_i \nabla(\log \rho_i + V_i)) + \sum_{r \in R} \left(k_r^{\text{fw}} \prod_{\bar{i} \in I} \rho_{\bar{i}}^{\alpha_{\bar{i}}^r} - k_r^{\text{bw}} \prod_{\bar{i} \in I} \rho_{\bar{i}}^{\beta_{\bar{i}}^r} \right) (\beta_i^r - \alpha_i^r), \quad \rho_i(0) := \rho_i^0. \quad (1.1)$$

where $\rho_i = \rho_i(t, x)$ describes the concentration of species X_i . The parameters characterizing the diffusion are the diffusion coefficients $\delta_i > 0$ and additional continuous drift potentials V_i . The chemical reactions are prescribed by forward and backward reaction rates $k_r^{\text{fw}}, k_r^{\text{bw}} > 0$, $r \in R$, and stoichiometric coefficients $\alpha_i^r, \beta_i^r \in [0, \infty)$ that describe the change of particles of different type, say X_i , by the chemical reactions

$$\forall r \in R: \quad \alpha_1^r X_1 + \dots + \alpha_{i_*}^r X_{i_*} \rightleftharpoons \beta_1^r X_1 + \dots + \beta_{i_*}^r X_{i_*}.$$

For simplicity, we consider the system on the d -dimensional torus \mathbb{T}^d , though an extension to bounded domains with homogeneous Neumann boundary conditions should not pose a significant difficulty.

The well-posedness, the long-time behavior, and approximations of systems of the form (1.1) have been studied with different methods for a long time. We refer to [Ali79, Rot06, Mor89, DF*07] and references therein for the study of classical solutions, i.e., solutions that are globally uniformly bounded in $L^\infty([0, \infty) \times \mathbb{T}^d; \mathbb{R}^I)$. In this context, two often used strategies are to obtain bounds for the full reaction-diffusion system by exploiting global a priori bounds for a lower order functional such as mass conservation or entropy bounds (cf. [Ali79, Mor89]) or by studying the space-independent reaction ODE system, which is applicable when all the species ρ_i , $i \in I$ diffuse with the same speed $\delta = \delta_i$.

However, to the surprise of many, in [PiS00] it was shown that in the case where species diffuse with different diffusion constants δ_i , there may exist no classical solutions to the reaction-diffusion system even when the involved reactions behave nicely. This furthered the interest in weaker notions of solutions, like renormalized solutions studied e.g. in [Fis15, Fis17].

In recent years, entropy methods became an important tool for the study of reaction-diffusion systems [DeF06, DF*07, DeF15, MHM15, DFT17]. Here, the idea is to use the non-increasing relative Boltzmann entropy (also called free energy) as an a priori bound to control solutions and study their long-time behavior. Moreover, entropy methods are a useful tool for deriving convergence results for the spatial discretization of linear reaction-diffusion systems, see e.g. [HPS24]; and it is the purpose of this work to generalize these results to nonlinear reaction kinetics.

We stress that our works main focus is not on the regularity of the spatial discretization nor of the model (like data or coefficients), but instead the variational nature of our approach, which is based on the theory of generalized gradient flows (see e.g. [Mie23] for an introduction).

To be more precise, we are interested in reaction-diffusion systems, where not only the free energy is decaying, but where the system is a *gradient flow* of the free energy. Starting with the pioneering work of Otto [JKO98, Ott01], it is known that many diffusion-type problems can be understood as gradient flows driven by a suitable free energy. Later, this was extended to reaction-diffusion systems satisfying *detailed balance* in [Mie11, LiM13, LMS16] for quadratic dissipations and in [MP*17] for cosh-type dissipations, which we also use here. The fundamental assumption here, is that the system satisfies the detailed balance (or reversibility) condition. This means that there exist reference concentrations $\omega = (\omega_i)_{i \in I}$ such that $\omega_i := \exp(-V_i)$ and such that for all $r \in R$ it holds

$$k_r^{\text{fw}} \prod_{\bar{i} \in I} \omega_{\bar{i}}^{\alpha_{\bar{i}}^r} = k_r^{\text{bw}} \prod_{\bar{i} \in I} \omega_{\bar{i}}^{\beta_{\bar{i}}^r} =: \kappa_r \prod_{\bar{i} \in I} \omega_{\bar{i}}^{\frac{\alpha_{\bar{i}}^r + \beta_{\bar{i}}^r}{2}}.$$

We observe that the detailed balance assumption ensures that the reaction-diffusion system (1.1) can now be written in the symmetric form

$$\partial_t \rho_i = \delta_i \operatorname{div} \left(\rho_i \nabla \log \left(\frac{\rho_i}{\omega_i} \right) \right) + \sum_{r \in R} \kappa_r \omega^{\frac{\alpha_r + \beta_r}{2}} \left(\left(\frac{\rho}{\omega} \right)^{\alpha_r} - \left(\frac{\rho}{\omega} \right)^{\beta_r} \right) (\beta_i^r - \alpha_i^r), \quad (1.2)$$

where we introduced the notation

$$\rho^{\alpha^r} := \prod_{i \in I} \rho_i^{\alpha_i^r},$$

which will be used throughout. We further note that (1.2) contains the *tilt-invariant* form of the reactions derived in [MiS20], where the dual dissipation potential, defined below, will not depend on ω .

What is more important to us, the system (1.2) has a gradient structure and can now be investigated with variational methods. More precisely, we will introduce continuous and discrete gradient systems in continuity equation format (cf. [PeS23]), link them to (1.2) and appropriate jump processes, respectively, and obtain a convergence result for these gradient systems in the spirit of Γ -convergence for gradient flows, see [SaS04], more precisely EDP-convergence in the sense of [MiS20, Ste21, MMP21, Mie23]. Upon rigorously linking these gradient systems to their corresponding equations, the finite approximation of solutions will then be a direct consequence.

Next, we discuss our finite approximation of the system (1.2). For simplicity, we discretize the torus using uniform grids \mathbb{Z}_N^d , $N \in \mathbb{N}$, noting that our model can be generalized to other domains and discretizations by following ideas of, e.g., [HrT23]. Furthermore, we assume for simplicity that the diffusion coefficients δ_i as well as the reaction coefficients κ_r are spatially independent, although our analysis would not be harmed when considering sufficiently smooth coefficients that are uniformly bounded above and away from zero.

For fixed $N \in \mathbb{N}$, the discretized evolution equation is a coupled ODE of the concentration $c_{i,k}$ of each species $i \in I$ in each discrete position $k \in \mathbb{Z}_N^d$. Denoting by $E := \{e = (e_1, \dots, e_d)^\top \in \{0, 1\}^d, \sum_{l=1}^d e_l = 1\}$ the set of d -dimensional unit vectors, the evolution is given by

$$\begin{aligned} \dot{c}_{i,k} = & \sum_{e \in E} \left[N^2 d_{i,k,e} \left(\frac{c_{i,k+e}}{w_{i,k+e}^N} - \frac{c_{i,k}}{w_{i,k}^N} \right) + N^2 d_{i,k,-e} \left(\frac{c_{i,k-e}}{w_{i,k-e}^N} - \frac{c_{i,k}}{w_{i,k}^N} \right) \right] \\ & + \sum_{r \in R} \kappa_r \omega^{\frac{\alpha_r + \beta_r}{2}} \left(\left(\frac{c_k}{w_k^N} \right)^{\alpha_r} - \left(\frac{c_k}{w_k^N} \right)^{\beta_r} \right) (\beta_i^r - \alpha_i^r), \end{aligned} \quad (1.3)$$

for the discrete reference concentrations $w_{i,k}^N := \int_{Q_k^N} \omega_i dx$, where $Q_k^N := \{x \in \mathbb{T}^d : x_l \in [k_l/N, (k_l+1)/N], l = 1, \dots, d\}$ are d -dimensional cubes of side length $1/N$. This system is related to the reaction-diffusion master equation (RDME) treated in [MSW23], where also the diffusion is replaced by jumps between nearest neighbors on the lattice. The intensity of the jumps is characterized by rates $d_{i,k,e} := \delta_i \sqrt{w_{i,k+e} w_{i,k}}$, which are scaled by N^2 . In our case, the reactions are modeled pointwise nonlinearities analogously to the space-continuous system, whereas in the RDME the reactions are modeled as linear jump processes on the number of particles. Our systems are complemented with suitable initial data satisfying a suitable well-preparedness condition specified later.

This work contains three main analytical results, which we summarize here. We refer to Section 4 for more details. The first main result, Theorem 4.3, is the rigorous link of each prelimit system (1.3) to a corresponding gradient structure via a so-called *energy-dissipation principle* (EDP). Here, the main step is proving a chain rule, which is obtained by exploiting the discrete nature of the underlying base space.

The second main result, Theorem 4.8, is the energy dissipation principle for the limit system (1.2). Since this model is defined over a continuous base space, multiple regularity issues have to be overcome in order to control in particular

the nonlinear reaction terms, which generate non-convexities in the variational formulation. Introducing the length $|\gamma|_1 = \sum_{i \in I} \gamma_i$ of stoichiometric vectors $\gamma \in [0, \infty)^I$, our main assumptions are the following:

$$\forall r \in R: \quad |\alpha^r|_1, |\beta^r|_1 \leq p_{\text{crit}} := 1+2/d \quad \text{and} \quad \frac{1}{2}|\alpha^r + \beta^r|_1 < p_{\text{crit}}. \quad (1.4)$$

Note that the same critical growth exponent p_{crit} appears already in [Mor89, Thm. 2.3] (one has to choose $a = 1$ there due to our L^1 bound obtained from the relative entropy) for showing global existence of smooth solutions.

The growth power p_{crit} can be achieved not only for solutions, but for all curves satisfying natural a priori bounds on the energy and dissipation by exploiting the regularity the diffusion provides. If the conditions (1.4) are not met, our analysis can still be carried out if the system admits natural L^∞ -bounds, see Remark 4.10. Such bounds are known to be satisfied by solutions to several classes of reaction-diffusion systems, namely if there exists a so-called bounding box, see [Smo94] and our Remark 4.10.

The final main result, Theorem 4.7, is the convergence of gradient systems. For this, we require the slightly weaker assumption than (1.4) that $\frac{1}{2}|\alpha^r + \beta^r|_1 \leq p_{\text{crit}}$ for all $r \in R$. The convergence proof consists of two parts, a compactness result and a lower limit. To establish the compactness, we construct a suitable family of embeddings into a unified space that crucially keep the gradient structure in tact.

With these three main results, the convergence of solutions of (1.3) to solutions of (1.2) follows in Corollary 4.9.

A major difficulty in the analysis of the space-continuous reaction-diffusion system comes from the reaction-induced nonlinearities and the resulting non-convexity of the dissipation. Here, we can use the some of the surprising properties of the cosh gradient structure based on the function $C^*(\zeta) = 4 \cosh(\zeta/2) - 4$, that is relevant for linear and nonlinear reactions, see [MP*17, LM*17, PeS23, MPS21, PR*22]. These surprising properties are encoded in nontrivial estimates for the Legendre dual C and its perspective function $\mathfrak{C} : (s, w) \mapsto wC(s/w)$, see (3.4). In particular, we can exploit the *magical estimate*

$$\forall q > 1 \forall s \in \mathbb{R} \forall w > 0: \quad C(s) \leq \frac{q}{q-1} \mathfrak{C}(s|w) + \frac{4w^q}{q-1} \quad (1.5)$$

(see 3.4d and Proposition A.1 for the proof). Note that such an estimate does not hold for dissipation potentials ψ of power-law type: for $\psi(s) = |s|^p$ with $p > 1$ we obtain $\Psi(s|w) = |s|^p/w^{p-1}$ such that the right-hand side in (1.5) only bounds the weaker power law $|s|^r$ with $r = pq/(p+q-1) \not\geq p$.

As usual, the chain rule is proved by a smoothing argument. In contrast to linear reaction systems like for Markov processes and Fokker-Planck type equations (cf. e.g., [Ste21, PeS23, PR*22]), it is not possible to rely solely on convexity arguments. Instead, our convergence proof combines the magical estimate with the Hardy-Littlewood maximal function from harmonic analysis and the easy but non-trivial estimate $|\partial_w \mathfrak{C}(s|w)| \leq 2|s/w|$ (see (3.4b)) to obtain an integrable majorant on the reactive flux. We believe that this flexible approach could also be used for handling non-convexities in other cases where the cosh gradient structure is relevant.

For the discrete approximation the challenge lies in deriving weak- L^1 compactness for the reactive fluxes. Here, we require p_{crit} -uniform integrability of the embedded concentrations. To achieve this, we exploit the flexibility of the embedding method by introducing a second family of more regular embeddings. For this family higher integrability can be obtained, while we rely on the first family of embeddings to obtain the liminf inequality.

The paper is structured as follows: In Section 2, we present the abstract strategy of the paper. Section 3 introduces first the gradient structures for the discrete and the continuous reaction-diffusion systems. Then, we connect both models with an embedding such that we can state the main results of the paper in Section 4. There, we also list and discuss in detail the assumptions on our reaction coefficients. The proof of our convergence result is carried out in Section 5. Here, we first derive the compactness, before showing the claimed liminf-estimate. Finally, Section 6 contains the detailed proofs of the chain rules inequality first for discrete and then for the continuous reaction-diffusion systems.

2 Abstract strategy

To improve clarity, before challenging the reader with the notation of our concrete problem, we first present on a formal and abstract level the strategy of our work.

2.1 Gradient systems with explicit abstract gradient mappings

We begin by introducing a quintuple $(X, Y, \mathbb{G}, \mathcal{E}, \mathcal{R}^*)$, called a *gradient system*. This notion is a small modification of gradient systems in continuity equation format introduced in [PeS23].

The elements of the gradient system are two pairs of *base spaces* $X = (X^{\text{dom}}, X^{\text{tar}})$, $Y = (Y^{\text{dom}}, Y^{\text{tar}})$, where $X^{\text{dom}}, Y^{\text{dom}}$ are Borel subsets of a Euclidean space, and $X^{\text{tar}}, Y^{\text{tar}}$ are Euclidean spaces. Test functions over these spaces are linked by an abstract linear *gradient map* $\mathbb{G} : C_c^\infty(X^{\text{dom}}, X^{\text{tar}}) \rightarrow C_c^\infty(Y^{\text{dom}}, Y^{\text{tar}})$, with dual $\mathbb{G}^* : (C_c^\infty(Y^{\text{dom}}, Y^{\text{tar}}))^* \rightarrow (C_c^\infty(X^{\text{dom}}, X^{\text{tar}}))^*$, which is sometimes called *process-space to tangent map*. Here, for $Z \in \{X, Y\}$ the dual pairing is defined as usual by

$$\forall \phi \in C_c^\infty(Z^{\text{dom}}, Z^{\text{tar}}) \quad \forall \mu \in (C_c^\infty(Z^{\text{dom}}, Z^{\text{tar}}))^* : \langle \phi, \mu \rangle_Z := \langle \phi, \mu \rangle := \int_{Z^{\text{dom}}} \phi \cdot d\mu,$$

with \cdot denoting the canonical inner product in the Euclidean space Z^{tar} .

The fourth element of the quintuple is a lower semicontinuous (lsc) *energy functional* $\mathcal{E} : \mathcal{M}_+(X^{\text{dom}}, X^{\text{tar}}) \rightarrow \mathbb{R} \cup \{\infty\}$, where $\mathcal{M}_+(X^{\text{dom}}, X^{\text{tar}})$ denotes the set of X^{tar} -valued, component-wise non-negative Radon measures. The final element is a *dual dissipation potential* $\mathcal{R}^* : \mathcal{M}_+(X^{\text{dom}}, X^{\text{tar}}) \times C(Y^{\text{dom}}, Y^{\text{tar}}) \rightarrow [0, \infty]$, which, by definition, is lsc and non-negative with $\mathcal{R}^*(\rho, 0) = 0$, and satisfies for all $\rho \in \mathcal{M}_+(X^{\text{dom}}, X^{\text{tar}})$ that $\xi \mapsto \mathcal{R}^*(\rho, \xi)$ is convex.

Fixing an arbitrary time horizon $T > 0$ and an initial datum $\rho_0 \in \mathcal{M}_+(X^{\text{dom}}, X^{\text{tar}})$, the gradient system $(X, Y, \mathbb{G}, \mathcal{E}, \mathcal{R})$ induces on $[0, T]$ an evolution equation, the *gradient flow equation*

$$\partial_t \rho = \mathbb{G}^* \partial_\xi \mathcal{R}^*(\rho, -\mathbb{G}D\mathcal{E}(\rho)), \quad (2.1a)$$

$$\rho(0) = \rho_0, \quad (2.1b)$$

where $D\mathcal{E}$ denotes the variational derivative of \mathcal{E} and $\partial_\xi \mathcal{R}^*$ denotes the convex subdifferential of $\mathcal{R}^*(\rho, \cdot)$.

By specifying \mathcal{R}^* and \mathcal{E} , the gradient system contains more information than the gradient-flow equation. Indeed, it is well-known that the same gradient-flow equation can be derived from different gradient systems, each corresponding to a different physical setting, see [Mie23].

Before further discussing the link between gradient flow and gradient system, we comment on the relation of the presented notion of gradient flow with other notions.

Remark 2.1 (Link to other notions of gradient flow). *The presented notion is heavily influenced by the gradient systems in continuity equation format introduced in [PeS23], the only difference being the split of X and Y in a domain and a target space, which allows us to directly incorporate well-known objects like the classical gradient $\nabla : C^1(\mathbb{T}^d) \rightarrow C(\mathbb{T}^d; \mathbb{R}^d)$ into our framework. Furthermore, we observe that by setting $\mathbb{G} = \text{id}$, $Y = X$, $\mathcal{X} = \mathcal{M}_+(X)$ and $\mathcal{R}^*(\rho, \varphi) := \mathcal{R}^*(\rho, \mathbb{G}\varphi)$ for all ρ, φ , we recover the well-established notion of a gradient system $(\mathcal{X}, \mathcal{E}, \mathcal{R}^*)$ as introduced in [Mie23]. Choosing \mathcal{R}^* as a quadratic functional, we can also recover metric gradient systems and metric gradient flows in the spirit of [AGS08].*

To establish the link between the gradient system $(X, Y, \mathbb{G}, \mathcal{E}, \mathcal{R}^*)$ and the gradient flow equation (2.1), we split the latter into two parts: First, we introduce the *continuity equation*, which links a weak-* measurable curve $\rho : [0, T] \rightarrow \mathcal{M}_+(X^{\text{dom}}, X^{\text{tar}})$ with a weak-* measurable *curve of fluxes* $j : [0, T] \rightarrow \mathcal{M}(Y^{\text{dom}}, Y^{\text{tar}})$ by the relation (understood in the sense of distributions on $[0, T] \times X^{\text{dom}}$)

$$\partial_t \rho = \mathbb{G}^* j. \quad (2.2)$$

The set of curves (ρ, j) satisfying (2.2) is denoted by CE.

Secondly, given a pair $(\rho, j) \in \text{CE}$, we recover (2.1) if the initial condition (2.1b) holds and j satisfies (in the sense of measures) the *constitutive relation*

$$j = \partial_\xi \mathcal{R}^*(\rho, -\mathbb{G}D\mathcal{E}(\rho)). \quad (2.3)$$

One important link between a gradient system and its induced gradient flow is called the *energy-dissipation principle*. It is formally established as follows. We introduce the (*primal*) *dissipation potential* $\mathcal{R} : \mathcal{M}_+(X^{\text{dom}}, X^{\text{tar}}) \times \mathcal{M}(Y^{\text{dom}}, Y^{\text{tar}}) \rightarrow [0, \infty]$ as the convex dual of \mathcal{R}^* with respect to the second variable. Together CE, \mathcal{E} , \mathcal{R} and \mathcal{R}^* give rise to the *dissipation functional*

$$\mathcal{D}(\rho, j) := \begin{cases} \int_0^T \mathcal{R}(\rho, j) + \mathcal{R}^*(\rho, -\mathbb{G}D\mathcal{E}(\rho)) dt & \text{for } (\rho, j) \in \text{CE} \\ +\infty & \text{for } (\rho, j) \notin \text{CE}, \end{cases}$$

and the *energy-dissipation functional*

$$\mathcal{L}(\rho, j) := \mathcal{E}(\rho(T)) - \mathcal{E}(\rho(0)) + \mathcal{D}(\rho, j).$$

We say that the gradient system satisfies the *energy-dissipation principle* if ρ solving (2.1) (in a suitable weak sense) is equivalent to (ρ, j) solving CE and $\mathcal{L}(\rho, j) = 0$.

A crucial role in making this principle rigorous is played by the *chain rule inequality* for the gradient system, which means that $\mathcal{L}(\rho, j) \geq 0$ holds for all $(\rho, j) \in \text{CE}$. This name is motivated by the following formal calculation:

$$\frac{d}{dt} \mathcal{E}(\rho) = \langle D\mathcal{E}(\rho), \partial_t \rho \rangle_X = -\langle -\mathbb{G}D\mathcal{E}(\rho), j \rangle_Y \geq -\mathcal{R}^*(\rho, -\mathbb{G}D\mathcal{E}(\rho)) - \mathcal{R}(\rho, j),$$

where the first equality is the classical chain rule, the second equality holds for $(\rho, j) \in \text{CE}$, and the inequality follows from the duality of \mathcal{R}^* and \mathcal{R} (Young-Fenchel estimate). Integrating in time from 0 to T , we obtain $\mathcal{L}(\rho, j) \geq 0$.

However, if $\mathcal{L}(\rho, j) \leq 0$ is imposed additionally, then we must have equality in the Young-Fenchel inequality for a.a. $t \in [0, T]$:

$$\langle -\mathbb{G}D\mathcal{E}(\rho), j \rangle_Y = \mathcal{R}^*(\rho, -\mathbb{G}D\mathcal{E}(\rho)) + \mathcal{R}(\rho, j).$$

By the Fenchel equivalence, this implies that (2.3) holds a.e. on $[0, T]$. Plugging this into CE (2.2) shows that (2.1) holds. The opposite direction from (2.1) to $\mathcal{L}(\rho, j) = 0$ with j from (2.1) is obvious.

Of course, we will make these arguments rigorous for the reaction-diffusion systems under consideration.

2.2 Convergence of gradient systems

Having introduced abstract gradient systems and briefly discussed the energy-dissipation principle, we now want to discuss, on an abstract level, our strategy for obtaining the convergence of gradient flows.

To this end, consider a family of approximating gradient systems $(X_N, Y_N, \mathbb{G}_N, \mathcal{E}_N, \mathcal{R}_N^*)_{N \in \mathbb{N}}$ inducing CE_N , \mathcal{D}_N , and \mathcal{L}_N as before. As a first step, one proves that each $(X_N, Y_N, \mathbb{G}_N, \mathcal{E}_N, \mathcal{R}_N^*)$ satisfies a chain rule inequality and an energy-dissipation principle. Next, one shows that for each $N \in \mathbb{N}$ and each initial datum ρ_N^0 with $\mathcal{E}_N(\rho_N^0) < \infty$ there exists a solution pair $(\tilde{\rho}_N, \tilde{j}_N) \in \text{CE}_N$ with $\tilde{\rho}_N(0) = \rho_N^0$ and $\mathcal{L}_N(\tilde{\rho}_N, \tilde{j}_N) = 0$.

Our aim is to connect the approximating gradient systems with a limit gradient system $(X, Y, \mathbb{G}, \mathcal{E}, \mathcal{R}^*)$ inducing CE, \mathcal{D} , and \mathcal{L} . For this, one has to show that $(X, Y, \mathbb{G}, \mathcal{E}, \mathcal{R}^*)$ also satisfies chain rule inequality and energy-dissipation principle.

To establish the link, a candidate curve that might be a solution for the limit system needs to be obtained by applying a compactness argument to the family of prelimit solutions $(\tilde{\rho}_N, \tilde{j}_N)_{N \in \mathbb{N}}$. However, the different gradient systems are defined over different base spaces, hence a unified space is needed in which compactness can be realized. To this end, one constructs an *embedding operator* $\iota_N : \mathcal{M}_+(X_N^{\text{dom}}, X_N^{\text{tar}}) \rightarrow \mathcal{M}_+(X^{\text{dom}}, X^{\text{tar}})$ and a *discretization operator* $\iota_N^* : C_c^\infty(X^{\text{dom}}, X^{\text{tar}}) \rightarrow C_c^\infty(X_N^{\text{dom}}, X_N^{\text{tar}})$ such that for all $\varphi \in C_c^\infty(X^{\text{dom}}, X^{\text{tar}})$ it holds

$$\langle \iota_N \rho_N, \varphi \rangle_X = \langle \rho_N, \iota_N^* \varphi \rangle_{X_N}.$$

For the fluxes one constructs $\iota_{N, \mathbb{G}} : \mathcal{M}_+(Y_N^{\text{dom}}, Y_N^{\text{tar}}) \rightarrow \mathcal{M}_+(Y^{\text{dom}}, Y^{\text{tar}})$ such that for all $\varphi \in C_c^\infty(X^{\text{dom}}, X^{\text{tar}})$ it holds

$$\langle \iota_{N, \mathbb{G}} j_N, \mathbb{G} \varphi \rangle_Y = \langle j_N, \mathbb{G}_N \iota_N^* \varphi \rangle_{Y_N}.$$

Since the continuity equation is understood in the sense of distributions, this implies that $(\rho_N, j_N) \in \text{CE}_N$ if and only if $(\iota_N \rho_N, \iota_{N, \mathbb{G}} j_N) \in \text{CE}$.

We can now prove that for each family $(\rho_N, j_N)_{N \in \mathbb{N}}$ with $(\rho_N, j_N) \in \text{CE}_N$ and $\sup_{N \in \mathbb{N}} \sup_{t \in [0, T]} \mathcal{E}_N(\rho_N(t)) < \infty$ as well as $\sup_{N \in \mathbb{N}} \mathcal{D}_N(\rho_N, j_N) < \infty$, there exists $(\rho, j) \in \text{CE}$ with $\mathcal{E}(\rho(0)) < \infty$ and $\mathcal{D}(\rho, j) < \infty$ such that (along a subsequence) $(\iota_N \rho_N, \iota_{N, \mathbb{G}} j_N) \rightharpoonup^* (\rho, j)$. In particular, such a limit $(\tilde{\rho}, \tilde{j})$ exists for the family $(\tilde{\rho}_N, \tilde{j}_N)_{N \in \mathbb{N}}$.

Next, one shows that for each family $(\rho_N, j_N)_{N \in \mathbb{N}}$ satisfying the a priori bounds as before and each limit (ρ, j) of the embedded family, we have the liminf estimates

$$\liminf_{N \rightarrow \infty} \mathcal{D}_N(\rho_N, j_N) \geq \mathcal{D}(\rho, j) \quad \text{and} \quad \liminf_{N \rightarrow \infty} \mathcal{E}_N(\rho_N(t)) \geq \mathcal{E}(\rho(t)) \quad \forall t \in [0, T]. \quad (2.4)$$

Notice that this inequality relates the dissipation functionals of the non-embedded curves with the limiting dissipation functional of the limiting curve. In particular, (2.4) holds for the previously obtained family of solutions $(\tilde{\rho}_N, \tilde{j}_N)_{N \in \mathbb{N}}$ and each of its limits $(\tilde{\rho}, \tilde{j})$.

To conclude that the limits are indeed solution, we now assume the well-preparedness of initial data

$$\iota_N \rho_N^0 \rightharpoonup^* \rho^0 \quad \text{and} \quad \lim_{N \rightarrow \infty} \mathcal{E}_N(\rho_N^0) = \mathcal{E}(\rho^0) < \infty.$$

The energy identity combined with (2.4) and the limit chain rule inequality yield

$$0 = \liminf_{N \rightarrow \infty} \mathcal{L}_N(\tilde{\rho}_N, \tilde{j}_N) \geq \mathcal{L}(\tilde{\rho}, \tilde{j}) \geq 0,$$

from which the energy-dissipation principle of the limit gradient system implies that $\tilde{\rho}$ is solution starting at $\tilde{\rho}(0) = \rho^0$ and that \tilde{j} is given by the kinetic relation (2.3).

3 Gradient system for the reaction-diffusion system

We want to describe the evolution of i_* chemical species X_i with $i \in \{1, \dots, i_*\} =: I$ undergoing diffusion in a subdomain $\Omega \subset \mathbb{R}^d$ and interacting according to r_* chemical reactions:

$$\sum_{i \in I} \alpha_i^r X_i \rightleftharpoons \sum_{i \in I} \beta_i^r X_i, \quad r \in \{1, \dots, r_*\} =: R.$$

Throughout the paper we assume that the physical domain is given by $\Omega = \mathbb{T}^d$ (the d -dimensional torus), and that we have finitely many species and reactions, i.e., $i_*, r_* \in \mathbb{N}$. In the following, we will also use the effective stoichiometric vectors $\gamma^r =: \alpha^r - \beta^r \in \mathbb{R}^I$. Moreover, we fix reaction coefficients $\kappa_r > 0$ (describing the reaction speed) for each reaction and diffusion coefficients $\delta_i > 0$ for each species.

3.1 Discrete reaction-diffusion gradient systems

We present the gradient structure for the spatially discrete reaction-diffusion system with fixed $N \in \mathbb{N}$. Denoting by $\mathbb{Z}_N^d = (\mathbb{Z}/N\mathbb{Z})^d$ the set of discrete positions (with periodic boundary conditions), and $E := \{e = (e_1, \dots, e_d)^\top \in \{0, 1\}^d, \sum_{l=1}^d e_l = 1\}$ the set of discrete directions, we introduce the spaces

$$\begin{aligned} X_N &:= (X_N^{\text{dom}}, X_N^{\text{tar}}) && := (I \times \mathbb{Z}_N^d, \mathbb{R}), \\ Y_{N,\text{diff}} &:= (Y_{N,\text{diff}}^{\text{dom}}, X_{N,\text{diff}}^{\text{tar}}) && := (I \times \mathbb{Z}_N^d \times E, \mathbb{R}), \\ Y_{N,\text{react}} &:= (Y_{N,\text{react}}^{\text{dom}}, X_{N,\text{react}}^{\text{tar}}) && := (R \times \mathbb{Z}_N^d, \mathbb{R}), \\ Y_N &:= (Y_N^{\text{dom}}, Y_N^{\text{tar}}) && := (Y_{N,\text{diff}}^{\text{dom}} \times Y_{N,\text{react}}^{\text{dom}}, Y_{N,\text{diff}}^{\text{tar}} \times Y_{N,\text{react}}^{\text{tar}}). \end{aligned}$$

We introduce the short notation $C(X_N) := C(X_N^{\text{dom}}; X_N^{\text{tar}})$ and analogously for all other spaces of functions/measures over these spaces. Furthermore, given a time interval $[0, T]$ we write $C([0, T] \times X_N) := C([0, T] \times X_N^{\text{dom}}; X_N^{\text{tar}})$ and analogously for all other spaces of functions or measures over these spaces.

Abusing notation, we denote by $\langle \cdot, \cdot \rangle_N$ the dual products for vectors as well as components, e.g., for $(\zeta, \xi) \in C(Y_N)$ and $(u, v) \in \mathcal{M}(Y_N)$ we write

$$\begin{aligned} \langle (\xi, \zeta), (u, v) \rangle_N &= \langle \xi, u \rangle_N + \langle \zeta, v \rangle_N = \sum_{i \in I} \langle \xi_i, u_i \rangle_N + \sum_{r \in R} \langle \zeta_r, v_r \rangle_N \\ &= \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \left(\sum_{i \in I} \sum_{e \in E} \xi_{i,k,e} u_{i,k,e} + \sum_{r \in R} \zeta_{r,k} v_{r,k} \right) \end{aligned}$$

and similarly for other functions/measures defined over X_N or Y_N .

Again abusing notation, but highlighting that no spatial component is involved, we introduce for the inner products on \mathbb{R}^I and \mathbb{R}^R the notation

$$\gamma \bullet \xi = \sum_{i \in I} \gamma_i \xi_i, \quad f \bullet \psi = \sum_{r \in R} f_r \psi_r.$$

Given stoichiometric vectors $\alpha^r, \beta^r \in [0, \infty)^I$ and $\gamma^r = \alpha^r - \beta^r$ for $r \in R$, we define the *discrete gradient* $\overline{\nabla}$, the *stoichiometric matrix* (or *Wegscheider matrix*) Γ , and the *abstract linear gradient map* $\overline{\mathbb{G}}$ by

$$\begin{aligned} \overline{\mathbb{G}} : C_c^\infty(X_N) &\rightarrow C_c^\infty(Y_N), & \overline{\mathbb{G}}\varphi &:= (\overline{\nabla}\varphi, \Gamma\varphi), \quad \text{with} \\ \overline{\nabla} : C_c^\infty(X_N) &\rightarrow C_c^\infty(Y_{N,\text{diff}}), & \overline{\nabla}\varphi_{i,k,e} &:= \varphi_{i,k+e} - \varphi_{i,k}, \quad \text{and} \\ \Gamma : C_c^\infty(X_N) &\rightarrow C_c^\infty(Y_{N,\text{react}}), & \Gamma\varphi_{r,k} &:= \sum_{i \in I} \gamma_i^r \varphi_{i,k} = \gamma^r \bullet \varphi_k. \end{aligned}$$

Their dual operators are given by

$$\begin{aligned} \overline{\mathbb{G}}^* : (C_c^\infty(Y_N))^* &\rightarrow (C_c^\infty(X_N))^*, & \overline{\mathbb{G}}^*(\xi, \zeta) &:= -\overline{\text{div}}\xi + \Gamma^*\zeta, \quad \text{with} \\ -\overline{\text{div}} : (C_c^\infty(Y_{N,\text{diff}}))^* &\rightarrow (C_c^\infty(X_N))^*, & -\overline{\text{div}}\xi_{i,k} &:= \sum_{e \in E} (\xi_{i,k-e,e} - \xi_{i,k,e}), \quad \text{and} \\ \Gamma^* : (C_c^\infty(Y_{N,\text{react}}))^* &\rightarrow (C_c^\infty(X_N))^*, & \Gamma^*\zeta_{i,k} &:= \sum_{r \in R} \gamma_i^r \zeta_{r,k} = \gamma_i \bullet \zeta_k. \end{aligned}$$

Elements of the state space $\mathcal{M}_+(X_N)$ are denoted by $c = (c_{i,k})_{i \in I, k \in \mathbb{Z}_N^d}$ and will be called *chemical concentrations*. We consider the *relative entropy* with respect to a positive *reference concentration* $w \in \mathcal{M}_+(X_N)$

$$E_N(c) := \frac{1}{N^d} \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} \lambda_B \left(\frac{c_{i,k}}{w_{i,k}} \right) w_{i,k}, \quad (3.1)$$

where the Boltzmann function is defined by $\lambda_B(r) = r \log r - r + 1$.

The *discrete dual dissipation potential* $R_N^* : \mathcal{M}_+(X_N) \times C(Y_N) \rightarrow [0, \infty)$ consists of two parts, which correspond to the discrete diffusion (i.e. jumps) and reactions, respectively. It is defined for $c \in \mathcal{M}_+(X_N)$, $\xi \in C(Y_{N,\text{diff}})$, and $\zeta \in C(Y_{N,\text{react}})$ by

$$\begin{aligned} R_N^*(c, (\xi, \zeta)) &:= R_{N,\text{diff}}^*(c, \xi) + R_{N,\text{react}}^*(c, \zeta) \quad \text{with} \\ R_{N,\text{diff}}^*(c, \xi) &:= \frac{1}{N^d} \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} N^2 \delta_i(c_{i,k}, c_{i,k+e})^{1/2} C^*(\xi_{i,k,e}), \\ R_{N,\text{react}}^*(c, \zeta) &:= \frac{1}{N^d} \sum_{r \in R} \sum_{k \in \mathbb{Z}_N^d} \kappa_r (c_k^{\alpha^r} c_k^{\beta^r})^{1/2} C^*(\zeta_{r,k}), \end{aligned}$$

where $C^*(r) := 4 \cosh(r/2) - 4$. In the sequel we will write $R_N^*(c, \xi, \zeta)$ instead of $R_N^*(c, (\xi, \zeta))$, and analogously for similar objects depending on a configuration, a diffusive component, and a reactive component. Note that the diffusive part of the dissipation contains a factor N^2 that will provide the continuous diffusion in the limit $N \rightarrow \infty$. Note that E_N depends on $w \in \mathcal{M}_+(X_N)$, whereas R_N^* is independent of w , which is called *tilt-invariance* in [MiS20].

The previously defined objects form the discrete gradient system $(X_N, Y_N, \overline{\mathbb{G}}, E_N, R_N^*)$. The corresponding gradient flow equation is the discrete reaction-diffusion system (1.3).

Throughout we will make use of various properties of the function $C^*(r)$ characterizing R_N^* and its Legendre transform C . We gather these properties in the following lemma:

Lemma 3.1. *The convex function $C^* : \mathbb{R} \rightarrow [0, \infty)$ defined by*

$$C^*(\sigma) = 4 \cosh(\sigma/2) - 4$$

and its convex conjugate

$$C(s) := \sup_{\sigma \in \mathbb{R}} \{\sigma s - C^*(\sigma)\} = 2s \text{Arsinh}(s/2) - 2\sqrt{s^2+4} + 4$$

have the following properties:

$$\begin{aligned} \forall a, b > 0 : \quad \sqrt{ab} \cdot C^*(\log a - \log b) &= 2|\sqrt{a} - \sqrt{b}|^2, \\ \sqrt{ab} \cdot (C^*)'(\log a - \log b) &= a - b; \end{aligned} \quad (3.2a)$$

$$\forall s \in \mathbb{R} : \quad C(s) \leq sC'(s) \leq 2C(s) \quad \text{and} \quad \frac{|s|}{2} \log(1+|s|) \leq C(s) \leq |s| \log(1+|s|). \quad (3.2b)$$

Proof. These results are obtained by elementary calculations, see e.g. [HrT23, Lem. 3.4] for more details. \square

In addition to \mathbb{C} we also need its so-called *perspective function* $\mathbb{C} : \times [0, \infty) \rightarrow [0, \infty]$, which is given by

$$\mathbb{C}(s|w) := \sup_{\zeta \in \mathbb{R}} \{s\zeta - w\mathbb{C}^*(\zeta)\} = \begin{cases} w\mathbb{C}(s/w) & \text{for } w > 0, \\ \chi_0(s) & \text{for } w = 0. \end{cases} \quad (3.3)$$

In the sequel we will need the following properties of \mathbb{C} . The last result is the magical estimate that will be crucially used in Proposition 6.3. For a similar estimate for the relative Boltzmann entropy, we refer to [FH*22, Eqn. (2.7)].

Lemma 3.2 (Properties of the perspective function \mathbb{C}).

$$\text{The mapping } \mathbb{R} \times [0, \infty) \ni (s, w) \mapsto \mathbb{C}(s|w) \text{ is strictly convex.} \quad (3.4a)$$

$$\left. \begin{aligned} \forall s \in \mathbb{R} : \quad w \mapsto \mathbb{C}(s|w) \text{ is non-increasing with} \\ \partial_w \mathbb{C}(s|w) = \mathbb{C}(r) - r\mathbb{C}'(r) \Big|_{r=s/w} = 4 - 2\sqrt{(s/w)^2 + 4} \leq 0. \end{aligned} \right\} \quad (3.4b)$$

$$\forall s \in \mathbb{R} \forall w > 0 : \quad (0, \infty) \ni \lambda \mapsto \mathbb{C}(\lambda s | \lambda^2 w) \text{ is increasing.} \quad (3.4c)$$

$$\forall q > 1 : \quad \mathbb{C}(s) \leq \frac{q}{q-1} \mathbb{C}(s|w) + \frac{4w^q}{q-1}. \quad (3.4d)$$

Proof. Property (3.4a) follows from the fact that $\mathbb{C}(\cdot|w)$ is the Legendre-Fenchel transform of $(\zeta, w) \mapsto w\mathbb{C}^*(\zeta)$ which is convex in ζ and concave in w .

The relation in (3.4b) follow by a direct computation using the lower estimate for $s\mathbb{C}'(s)$ in (3.2b). Assertion (3.4c) follows by using the upper bound for $s\mathbb{C}'(s)$ in (3.2b). For the proof of the magical estimate (3.4d) we refer to Appendix A. \square

We call (3.4d) the *magical estimate for \mathbb{C} and its perspective function* \mathbb{C} , since such an estimate cannot be expected from general dissipation functions. For instance, for $\Phi : s \mapsto c_1|s|^q$ with $q > 1$ the infimum of $w\Phi(s/w) + c_2w^p$ only provides an upper bound for $s \mapsto c_3|s|^r$ with $r = qp/(p+q-1) \not\leq q$. The magical estimate (3.4d) will be important for proving the chain rule, see the proof of Theorem 4.8 in Section 6.2.

As a weaker replacement of (3.4d) we will need the following result that is proved in Appendix B.

Lemma 3.3 (Superliner estimates). *Consider an even, differentiable, and superlinear function $\phi : \mathbb{R} \rightarrow [0, \infty)$ such that $s\phi'(s) \geq \phi(s)$ and another non-decreasing superlinear function $\psi : [0, \infty) \rightarrow [0, \infty)$. Then, the function $\Xi_{\phi, \psi} : \mathbb{R} \rightarrow [0, \infty)$ defined via*

$$\Xi_{\phi, \psi}(s) := \inf_{w > 0} \{w\phi(s/w) + \psi(w)\},$$

is even, non-decreasing and superlinear.

For $c > 0$, the dual dissipation potential induces a slope term by the relation $S_N(c) = R_N^*(c, -\overline{\mathbb{G}}DE_N(c))$. This definition can then be extended to all $c \in \mathcal{M}_+(X_N)$ (cf. [LaS24, Remark 3.7]) by exploiting the identity (3.2a) for \mathbb{C}^* and \log . This yields the so-called *relaxed slope*.

Definition 3.4 (Relaxed slope). *The relaxed slope $S_N : \mathcal{M}_+(X_N) \rightarrow [0, \infty)$ is defined by*

$$\begin{aligned} S_N(c) &:= S_{N, \text{diff}}(c) + S_{N, \text{react}}(c), \\ S_{N, \text{diff}}(c) &:= \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \sum_{i \in I} \sum_{e \in E} 2\delta_i N^2 \sqrt{w_{i, k+e} w_{i, k}} \left(\sqrt{\frac{c_{i, k+e}}{w_{i, k+e}}} - \sqrt{\frac{c_{i, k}}{w_{i, k}}} \right)^2, \\ S_{N, \text{react}}(c) &:= \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \sum_{r \in R} 2\kappa_r \sqrt{w_k^{\alpha r} w_k^{\beta r}} \left(\left(\frac{c_k}{w_k} \right)^{\alpha r/2} - \left(\frac{c_k}{w_k} \right)^{\beta r/2} \right)^2. \end{aligned}$$

Next, we introduce the primal dissipation potential R_N .

Definition 3.5 (Primal dissipation potential). *We define the primal dissipation potential $R_N : \mathcal{M}_+(X_N) \times \mathcal{M}(Y_{N,\text{diff}}) \times \mathcal{M}(Y_{N,\text{react}}) \rightarrow [0, \infty)$ for $c \in \mathcal{M}_+(X_N)$, $F \in \mathcal{M}(Y_{N,\text{diff}})$, and $J \in \mathcal{M}(Y_{N,\text{react}})$ by*

$$\begin{aligned} R_N(c, F, J) &:= R_{N,\text{diff}}(c, F) + R_{N,\text{react}}(c, J), \\ R_{N,\text{diff}}(c, F) &:= \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \sum_{i \in I} \sum_{e \in E} \mathfrak{C} \left(F_{i,k,e}^N \left| N^2 \delta_i (c_{i,k}^N c_{i,k+e}^N)^{1/2} \right. \right), \\ R_{N,\text{react}}(c, J) &:= \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \sum_{r \in R} \mathfrak{C} \left(J_{r,k}^N \left| \kappa_r (c_k^N)^{(\alpha_r + \beta_r)/2} \right. \right). \end{aligned}$$

Note that R_N is the convex conjugate of R_N^* with respect to the second and third arguments. Indeed, the dualities $(R_{N,\text{diff}}^*)^* = R_{N,\text{diff}}$ and $(R_{N,\text{react}}^*)^* = R_{N,\text{react}}$ follow from the duality of \mathfrak{C} and \mathfrak{C}^* . The duality of the sums then follows from the fact that the summands are independent of each other.

Definition 3.6 (Energy-dissipation functional). *We introduce the dissipation functional $D_N : L^1(0, T; \mathcal{M}_+(X_N) \times \mathcal{M}(Y_{N,\text{diff}}) \times \mathcal{M}(Y_{N,\text{react}})) \rightarrow [0, \infty]$ by*

$$D_N(c, F, J) := \int_0^T \{R_N(c(t), F(t), J(t)) + S_N(c(t))\} dt. \quad (3.5)$$

Furthermore, we introduce the energy-dissipation functional

$$L_N(c, F, J) := E_N(c(T)) - E_N(c(0)) + D_N(c, F, J).$$

Definition 3.7 (Continuity equation). *The operator $\overline{\mathbb{G}}$ gives rise to the continuity equation*

$$\dot{c} = \overline{\mathbb{G}}^*(F, J) = -\overline{\text{div}} F + \Gamma^* J.$$

We denote $\overline{\text{CE}}_N$ the set of triples $(c, F, J) \in AC([0, T]; \mathcal{M}(X_N)) \times L^1(0, T; \mathcal{M}(Y_{N,\text{diff}})) \times L^1(0, T; \mathcal{M}(Y_{N,\text{react}}))$ satisfying the above equation.

In this definition the domains of the sets X_N , $Y_{N,\text{diff}}$, and $Y_{N,\text{react}}$ are finite sets, such that the topology for the measure spaces is irrelevant. Only in the continuous case, it will be important to use the narrow topology, see Definition 3.12. Moreover, following the proof of [Erb14, Lem. 3.1], we observe that this definition is indeed well-posed for F and J satisfying L^1 -bounds in time.

For further reference, we note that $(c, F, J) \in \overline{\text{CE}}_N$ if and only if for all $\varphi \in C(X_N)$ and all $k \in \mathbb{Z}_N^d$ and a.e. $t \in [0, T]$ it holds

$$\frac{d}{dt} \left[\sum_{i \in I} \varphi_{i,k} c_{i,k} \right] = \sum_{i \in I} \sum_{e \in E} (\overline{\nabla} \varphi)_{i,k,e} F_{i,k,e} + \sum_{r \in R} (\Gamma \varphi)_{r,k} J_{r,k}.$$

We conclude this section by specifying our notion of solution for (1.3). For the subsequent analysis, it will be crucial to use already the notion of *energy-dissipation balance solutions* (in short EDB solutions) that are based on the energy-dissipation functional L_N . Theorem 4.3 will provide a rigorous connection between this notion and the ODE system (1.3) based on the corresponding chain rule as explained in Section 2.1. Even in this finite-dimensional case, this equivalence is non-trivial.

Definition 3.8 (Discrete EDB solutions). *We say $c \in AC([0, T]; \mathcal{M}_+(X_N))$ is a discrete EDB solution of (1.3) with initial datum $c_0 \in \mathcal{M}_+(X_N)$, if $c(0) = c_0$ and if there exists (F, J) such that $(c, F, J) \in \overline{\text{CE}}_N$ and for $0 \leq s < t \leq T$ we have*

$$L_N^{[s,t]}(c, F, J) := E_N(c(t)) - E_N(c(s)) + \int_s^t (R_N(c, F, J) + S_N(c)) dr = 0. \quad (3.6)$$

3.2 Continuous-space reaction-diffusion gradient system

We present the gradient structure for the reaction-diffusion system for the case of the ‘continuous space’ given by the torus \mathbb{T}^d ; as a short-hand we will use the name “*continuum system*”. The base spaces we consider are

$$\begin{aligned} X &:= (X^{\text{dom}}, X^{\text{tar}}) && := (\mathbb{T}^d, \mathbb{R}^I), \\ Y_{\text{diff}} &:= (Y_{\text{diff}}^{\text{dom}}, Y_{\text{diff}}^{\text{tar}}) && := (\mathbb{T}^d, (\mathbb{R}^d)^I), \\ Y_{\text{react}} &:= (Y_{\text{react}}^{\text{dom}}, Y_{\text{react}}^{\text{tar}}) && := (\mathbb{T}^d, \mathbb{R}^R), \\ Y &:= (Y^{\text{dom}}, Y^{\text{tar}}) && := (Y_{\text{diff}}^{\text{dom}} \times Y_{\text{react}}^{\text{dom}}, Y_{\text{diff}}^{\text{tar}} \times Y_{\text{react}}^{\text{tar}}). \end{aligned}$$

We recall the short notations $C(X) := C(X^{\text{dom}}, X^{\text{tar}})$ and $C([0, T] \times X) := C([0, T] \times X^{\text{dom}}, X^{\text{tar}})$ as well as analogous notations for all other spaces of functions/measures over these spaces.

Similar to before, we abuse notation, denoting by $\langle \cdot, \cdot \rangle$ the dual products for vectors as well as components, e.g., for $(\zeta, \xi) \in C(Y)$ and $(u, v) \in \mathcal{M}(Y)$ we write

$$\begin{aligned} \langle (\xi, \zeta), (u, v) \rangle &= \langle \xi, u \rangle_N + \langle \zeta, v \rangle = \sum_{i \in I} \langle \xi_i, u_i \rangle + \sum_{r \in R} \langle \zeta_r, v_r \rangle \\ &= \int_{\mathbb{T}^d} \left(\sum_{i \in I} \sum_{l=1}^d \xi_{i,l}(x) u_{i,l}(x) + \sum_{r \in R} \zeta_r(x) v_r(x) \right) dx, \end{aligned}$$

and similarly for other functions/measures defined over X or Y .

The notation for sums over I and R is used also in the continuous context:

$$\gamma \bullet \xi = \sum_{i \in I} \gamma_i \xi_i, \quad f \bullet \psi = \sum_{r \in R} f_r \psi_r.$$

Given stoichiometric vectors $\alpha^r, \beta^r \in [0, \infty)^I$, $\gamma^r = \alpha^r - \beta^r$, $r \in R$, we consider the (classical) gradient ∇ and the stoichiometric matrix Γ as well as the linear gradient map \mathbb{G} given by

$$\begin{aligned} \mathbb{G} : C_c^\infty(X) &\rightarrow C_c^\infty(Y), && \mathbb{G} \varphi := (\nabla \varphi, \Gamma \varphi) \quad \text{with} \\ \nabla : C_c^\infty(X) &\rightarrow C_c^\infty(Y_{\text{diff}}), && \nabla \varphi_i(x) := (\partial_{x_l} \varphi_i(x))_{l=1, \dots, d}, \\ \Gamma : C_c^\infty(X) &\rightarrow C_c^\infty(Y_{\text{react}}), && \Gamma \varphi_r(x) := \sum_{i \in I} \gamma_i^r \varphi_i(x) = \gamma^r \bullet \varphi(x). \end{aligned}$$

Their duals are given by

$$\begin{aligned} \mathbb{G}^* : (C_c^\infty(Y))^* &\rightarrow (C_c^\infty(X))^*, && \mathbb{G}^*(\xi, \zeta) := -\text{div } \xi + \Gamma^* \zeta \quad \text{with} \\ -\text{div} : (C_c^\infty(Y_{\text{diff}}))^* &\rightarrow (C_c^\infty(X))^*, && -\text{div } \xi_i(x) := -\sum_{l=1}^d \partial_{x_l} \xi_{i,l}(x), \\ \Gamma^* : (C_c^\infty(Y_{\text{react}}))^* &\rightarrow (C_c^\infty(X))^*, && \Gamma^* \zeta_r(x) := \sum_{i \in I} \gamma_i^r \zeta_i(x) = \gamma^r \bullet \zeta(x). \end{aligned}$$

Elements of the state space $\mathcal{M}_+(X)$ are denoted by ρ and will be called (*continuous-space*) *chemical concentrations*. In our situation the measures will always have a density with respect to the Lebesgue measure on \mathbb{T}^d , which (slightly abusing notation) will also be denoted by ρ .

We consider the *relative entropy* with respect to a *reference measure* $\omega \in \mathcal{M}_+(X)$

$$\mathcal{E}(\rho) = \sum_{i \in I} \int_{\mathbb{T}^d} \lambda_B \left(\frac{\rho_i}{\omega_i} \right) \omega_i dx, \quad (3.7)$$

where we recall the Boltzmann function $\lambda_B(r) = r \log r - r + 1$.

The *continuous dual dissipation potential* $\mathcal{R}^* : \mathcal{M}_+(X) \times C(Y) \rightarrow [0, \infty)$ is given for $\rho \in \mathcal{M}_+(X)$, $\xi \in C(Y_{\text{diff}})$, and $\zeta \in C(Y_{\text{react}})$ by

$$\begin{aligned}\mathcal{R}^*(\rho, (\xi, \zeta)) &:= \mathcal{R}_{\text{diff}}^*(\rho, \xi) + \mathcal{R}_{\text{react}}^*(\rho, \zeta), \\ \mathcal{R}_{\text{diff}}^*(\rho, \xi) &:= \sum_{i \in I} \frac{\delta_i}{2} \int_{\mathbb{T}^d} |\xi_i|^2 \rho_i \, dx, \\ \mathcal{R}_{\text{react}}^*(\rho, \zeta) &:= \sum_{r \in R} \kappa_r \int_{\mathbb{T}^d} (\rho^{\alpha^r} \rho^{\beta^r})^{1/2} \mathbb{C}^*(\zeta_r) \, dx.\end{aligned}$$

As in the discrete setting, from now on we will write $\mathcal{R}^*(\rho, \xi, \zeta)$ instead of $\mathcal{R}^*(\rho, (\xi, \zeta))$ and do the same for similar objects.

These objects form the continuous gradient system in continuity format $(X, Y, \mathbb{G}, \mathcal{E}, \mathcal{R}^*)$.

For $\rho > 0$ smooth, the dual dissipation potential induces a slope term by the relation $\mathcal{S}(\rho) = \mathcal{R}^*(\rho, -\mathbb{G} \mathcal{D}\mathcal{E}(\rho))$. This definition can then be extended to all $\rho \in \mathcal{M}_+(X)$ (cf. [HPS24, (3.24)]) yielding the relaxed slope.

Definition 3.9 (Relaxed slope). *The relaxed slope $\mathcal{S} : \mathcal{M}_+(X) \rightarrow [0, \infty)$ is defined by*

$$\begin{aligned}\mathcal{S}(\rho) &:= \mathcal{S}_{\text{diff}}(\rho) + \mathcal{S}_{\text{react}}(\rho), \\ \mathcal{S}_{\text{diff}}(\rho) &:= \sum_{i \in I} 2\delta_i \int_{\mathbb{T}^d} \left| \nabla \sqrt{\frac{\rho_i}{\omega_i}} \right|^2 \omega_i \, dx, \\ \mathcal{S}_{\text{react}}(\rho) &:= \sum_{r \in R} 2\kappa_r \int_{\mathbb{T}^d} \sqrt{\omega^{\alpha^r} \omega^{\beta^r}} \left(\left(\frac{\rho}{\omega} \right)^{\alpha^r/2} - \left(\frac{\rho}{\omega} \right)^{\beta^r/2} \right)^2 \, dx.\end{aligned}$$

Next, we introduce the primal dissipation potential $\mathcal{R} : \mathcal{M}_+(X) \times \mathcal{M}(Y) \rightarrow [0, \infty)$, which, as before, is given as the convex conjugate of \mathcal{R}^* with respect to the second argument.

Definition 3.10 (Primal dissipation potential). *The primal dissipation potential $\mathcal{R} : \mathcal{M}_+(X) \times \mathcal{M}(Y_{\text{diff}}) \times \mathcal{M}(Y_{\text{react}}) \rightarrow [0, \infty)$ is defined for $\rho \in \mathcal{M}_+(X)$, $f \in \mathcal{M}(Y_{\text{diff}})$, and $j \in \mathcal{M}(Y_{\text{react}})$ by*

$$\begin{aligned}\mathcal{R}(\rho, f, j) &:= \mathcal{R}_{\text{diff}}(\rho, f) + \mathcal{R}_{\text{react}}(\rho, j), \\ \mathcal{R}_{\text{diff}}(\rho, f) &:= \begin{cases} \sum_{i \in I} \frac{1}{2\delta_i} \int_{\mathbb{T}^d} \frac{|f_i|^2}{\rho_i} \, dx & \text{for } f_i = f_i \, dx \ll \mathcal{L}^d, \\ \infty & \text{otherwise,} \end{cases} \\ \mathcal{R}_{\text{react}}(\rho, j) &:= \begin{cases} \sum_{r \in R} \int_{\mathbb{T}^d} \mathbb{C}(j_r | \kappa_r (\rho^{\alpha^r} \rho^{\beta^r})^{1/2}) \, dx & \text{for } j_r = j_r \, dx \ll \mathcal{L}^d, \\ \infty & \text{otherwise,} \end{cases}\end{aligned}$$

where we again made a slight abuse of notation.

Definition 3.11 (Energy-dissipation functional). *We define the dissipation functional $\mathcal{D} : L^1(0, T; \mathcal{M}_+(X) \times \mathcal{M}(Y_{\text{diff}}) \times \mathcal{M}(Y_{\text{react}})) \rightarrow \mathbb{R}$ by*

$$\mathcal{D}(\rho, f, j) := \int_0^T \{ \mathcal{R}(\rho(t), f(t), j(t)) + \mathcal{S}(\rho(t)) \} \, dt. \quad (3.8)$$

Furthermore, we introduce the energy-dissipation functional

$$\mathcal{L}(\rho, f, j) := \mathcal{E}(\rho(T)) - \mathcal{E}(\rho(0)) + \mathcal{D}(\rho, f, j).$$

Definition 3.12 (Continuity equation). *The operator \mathbb{G} gives rise to the continuity equation*

$$\partial_t \rho = \mathbb{G}^*(f, j) = -\operatorname{div} f + \Gamma^* j.$$

We denote by CE the set of triples $(\rho, f, j) \in \operatorname{AC}([0, T]; \mathcal{M}_+(X)) \times L^1(0, T; \mathcal{M}(Y_{\text{diff}})) \times L^1(0, T; \mathcal{M}(Y_{\text{react}}))$ satisfying for all $\varphi \in C^1(X)$

$$\frac{d}{dt} \left[\int_{\mathbb{T}^d} \sum_{i \in I} \varphi_i \rho_i \, dx \right] = \int_{\mathbb{T}^d} \sum_{i \in I} \sum_{e \in E} (\nabla \varphi)_{i,e} f_{i,e} \, dx + \int_{\mathbb{T}^d} \sum_{r \in R} (\Gamma \varphi)_r j_r \, dx.$$

It is important here to recall that the absolute continuity in $AC([0, T]; \mathcal{M}_+(X))$ has to be understood with respect to a metric generating the narrow topology in $\mathcal{M}_+(X)$. Moreover, $L^1(0, T; \mathcal{M}(Y_{\text{diff}}))$ is meant to contain weakly measurable functions with $t \mapsto \|f(t)\|_{\mathcal{M}(Y_{\text{diff}})}$ lies in $L^1([0, T])$.

Combining the proofs of [AGS08, Lem. 8.1.2] and [Erb14, Lem. 3.1], we observe that this definition is well-posed for f and j satisfying L^1 -bounds.

We conclude this section by specifying our notion of solutions for the continuous-space reaction-diffusion gradient system (1.2).

Definition 3.13 (Continuum EDB solutions for (1.2)). *We say $\rho \in AC([0, T]; \mathcal{M}_+(X))$ is a continuum EDB solution of (1.2) if $\sup_{t \in [0, T]} \mathcal{E}(\rho(t)) < \infty$ and if there exists (f, j) such that $(\rho, f, j) \in \text{CE}$, $\mathcal{D}(\rho, f, j) < \infty$, and for $0 \leq s < t \leq T$ we have*

$$\mathcal{L}^{[s, t]}(\rho, f, j) := \mathcal{E}(\rho(t)) - \mathcal{E}(\rho(s)) + \int_s^t (\mathcal{R}(\rho, f, j) + \mathcal{S}(\rho)) \, dr = 0.$$

In the present paper, we will not show that all continuum EDB solutions ρ are weak solutions (in a suitable sense). However, under the additional assumption of positivity and boundedness for all ρ_i , Proposition 3.14 provides a result in this direction. Instead, we focus on the convergence of discrete EDB solutions c^N in the sense of Definition 3.8 to continuum EDB solutions. In fact, we establish the stronger EDP-convergence which also asks convergence of E_N to \mathcal{E} and D_N to \mathcal{D} .

The strategy is as explained in Section 2.2. By a limit passage we obtain $\mathcal{L}^{[0, T]}(\rho, f, j) \leq 0$, see the lower-limit estimates in Section 5. In Section 6 we establish the chain rule estimate $\mathcal{L}^{[s, t]}(\rho, f, j) \geq 0$ which then implies that ρ is a continuum EDB solution. In Section 4 we state the precise assumptions and results.

We close this subsection with stating a conditioned Energy-Dissipation Principle. If we have lower and upper bounds of the densities, then it follows that functions are continuum EDB solutions if and only if they are weak solutions.

Proposition 3.14 (Continuum EDB and weak solutions for (1.2)). *Consider concentrations $\rho \in H^1([0, T]; H^{-1}(\mathbb{T}^d)) \cap L^2([0, T]; H^1(\mathbb{T}^d))$ and $\sigma \in (0, 1)$ such that ρ satisfies $\rho_i(t, x) \in [\sigma, 1/\sigma]$ for all $i \in I$ and a.a. $(t, x) \in [0, T] \times \mathbb{T}^d$. Then, ρ is a weak solution of (1.2) if and only if $(\rho, f, j) \in \text{CE}$ with*

$$f_i = -\delta_i \nabla \rho_i \quad \text{and} \quad j_r = \kappa_r \omega^{(\alpha^r + \beta^r)/2} \left(\frac{\rho^{\alpha^r}}{\omega^{\alpha^r}} - \frac{\rho^{\beta^r}}{\omega^{\beta^r}} \right), \quad (3.9)$$

is a continuum EDB solution in the sense of Definition 3.13.

The proof is given in Section 6.2.

3.3 Embedding

As a crucial step for obtaining the convergence of gradient systems, we highlighted in Section 2.2 the construction of suitable embeddings connecting the prelimit spaces to the limit space.

Definition 3.15 (Embedding and discretization operators). *We introduce for each $k \in \mathbb{Z}_N^d$ the cube*

$$Q_k^N := \{x \in \mathbb{T}^d : x_l \in [k_l/N, (k_l + 1)/N], l = 1, \dots, d\}.$$

Next, we define the embedding operator $\iota_N : \mathcal{M}(X_N) \rightarrow \mathcal{M}(X)$ by

$$\iota_N(c_i)(x) := \rho_i(x) := \sum_{k \in \mathbb{Z}_N^d} c_{i,k} \mathbb{1}_{Q_k^N}(x).$$

Dual to it, we introduce the discretization operator $\iota_N^* : C(X) \rightarrow C(X_N)$ by setting

$$\iota_N^* \xi_{i,k} := (\iota_N^* \xi_i)_k := N^d \int_{Q_k^N} \xi_i \, dx.$$

For the diffusive fluxes we introduce $\iota_{N, \text{diff}} : \mathcal{M}_+(Y_{N, \text{diff}}) \rightarrow \mathcal{M}(Y_{\text{diff}})$ defined by

$$\iota_{N, \text{diff}} F_i(x) := f_i(x) = (f_{i, e_1}(x), \dots, f_{i, e_d}(x))^\top \quad (3.10a)$$

where for $e \in E$ we set

$$f_{i,e}(x) = \frac{1}{N} \sum_{k \in \mathbb{Z}_N^d} \left(\int_0^1 \mathbb{1}_{Q_{k+\theta e}^N}(x) d\theta \right) F_{i,k,e}. \quad (3.10b)$$

Finally, for the reactive fluxes we define $\iota_{N,\text{react}} : \mathcal{M}_+(Y_{N,\text{react}}) \rightarrow \mathcal{M}(Y_{\text{react}})$ by

$$\iota_{N,\text{react}} J_r(x) := j_r(x) := \sum_{k \in \mathbb{Z}_N^d} \mathbb{1}_{Q_k^N}(x) J_{r,k}. \quad (3.10c)$$

Using the above embedding operator is clear that $E_N(c) = \mathcal{E}(\iota_N(c))$ and analogous identities hold for other integral functionals as well. Moreover, by construction, $s \mapsto f_{i,e}(x+se)$ is piecewise affine, whereas $s \mapsto f_{i,e}(x+s\hat{e})$ is piecewise constant for $\hat{e} \neq e$. Moreover, by definition we have for all $i \in I$ and all $e \in E$ the estimate

$$\int_{\mathbb{T}^d} |f_{i,e}(x)| dx \leq \frac{1}{N} \int_0^1 \sum_{k \in \mathbb{Z}_N^d} \int_{\mathbb{T}^d} \mathbb{1}_{Q_{j+\theta e}^N}(x) dx d\theta |F_{i,k,e}| \leq \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \frac{|F_{i,k,e}|}{N}, \quad (3.11)$$

and for all $r \in R$ the estimate

$$\int_{\mathbb{T}^d} |j_r(x)| dx \leq \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} |J_{r,k}|.$$

Denoting the discrete L^1 -norms on $L^1(\mathbb{Z}_N^d)$ by $\|G\|_{L_N^1} := \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} |G_k|$, the estimates can be written equivalently as

$$\forall i \in I, e \in E: \quad \|f_{i,e}\|_{L^1} \leq \frac{1}{N} \|F_{i,e}\|_{L_N^1}, \quad \forall r \in R: \quad \|j_r\|_1 \leq \|J_r\|_{L_N^1}.$$

To simplify notation, for all $N \in \mathbb{N}$ and $y \in \mathbb{R}^d$ we introduce the *shift-operator* S_y^N defined by

$$S_y^N : L^1(\mathbb{T}^d) \rightarrow L^1(\mathbb{T}^d), \quad S_y^N \phi(x) := \phi\left(\left(x + \frac{y}{N}\right) \bmod 1\right), \quad (3.12)$$

where the modulus is applied componentwise.

The following lemma uses the embeddings defined above to connect the discrete and continuous continuity equations (recall $\overline{\text{CE}}_N$ from Definition 3.7).

Lemma 3.16. *For each $c \in \mathcal{M}_+(X_N)$, $\varphi \in C(X)$, it holds*

$$\langle \iota_N c, \varphi \rangle = \langle c, \iota_N^* \varphi \rangle_N.$$

Furthermore, we have for $\varphi \in C(X)$, $(F, J) \in \mathcal{M}(Y_N)$ that

$$\langle \iota_{N,\text{diff}} F, \nabla \varphi \rangle = \langle F, \overline{\nabla} \iota_N^* \varphi \rangle_N \quad \text{and} \quad \langle \iota_{N,\text{react}} J, \Gamma \varphi \rangle = \langle J, \Gamma \iota_N^* \varphi \rangle_N.$$

In particular, it holds $(c, F, J) \in \overline{\text{CE}}_N$ if and only if $(\iota_N c, \iota_{N,\text{diff}} F, \iota_{N,\text{react}} J) \in \text{CE}$.

Proof. For the first equality, we calculate

$$\langle \xi_i, \iota_N c_i \rangle = \int_{\mathbb{T}^d} \xi_i \sum_{k \in \mathbb{Z}_N^d} c_{i,k} \mathbb{1}_{Q_k^N} dx = \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \iota_N^* \xi_{i,k} c_{i,k} = \langle \iota_N^* (\xi_i), c_i \rangle_N.$$

Furthermore, we have for all test functions $\varphi \in C_0^\infty(X)$ that

$$\langle F, \overline{\nabla} \iota_N^* \varphi \rangle_N = \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} F_{k,e} \bullet [(\iota_N^* \varphi)_{k+e} - (\iota_N^* \varphi)_k] = \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} F_{k,e} \bullet \int_{Q_k^N} [S_e^N \varphi - \varphi] dx.$$

Rewriting for each $i \in I$ the integral by

$$S_e^N \varphi_i(x) - \varphi_i(x) = \int_0^1 \nabla \varphi_i \left(x + \frac{e}{N} \theta \right) \cdot \frac{e}{N} d\theta = \frac{1}{N} \int_0^1 S_{e\theta}^N \partial_{x_e} \varphi_i(x) d\theta, \quad (3.13)$$

and using Fubini for the integrable integrand, we get

$$\begin{aligned} \langle F, \bar{\nabla} \iota_N^* \varphi \rangle_N &= \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} \frac{F_{k,e}}{N} \bullet \int_{Q_k^N} \int_0^1 S_{e\theta}^N \partial_{x_e} \varphi(x) \, d\theta \, dx \\ &= \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} \frac{F_{k,e}}{N} \bullet \int_{\mathbb{T}^d} \mathbb{1}_{Q_k^N}(x) \int_0^1 S_{e\theta}^N \partial_{x_e} \varphi(x) \, d\theta \, dx \\ &= \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} \frac{F_{k,e}}{N} \bullet \int_{\mathbb{T}^d} \int_0^1 \mathbb{1}_{Q_{j+e\theta}^N}(x) \partial_{x_e} \varphi(x) \, d\theta \, dx = \int_{\mathbb{T}^d} \sum_{e \in E} f_e(x) \bullet \partial_{x_e} \varphi(x) \, dx = \langle f^N, \nabla \varphi \rangle. \end{aligned}$$

For the reactive flux, we simply observe that

$$\langle J, \Gamma \iota_N^* \varphi \rangle_N = \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} (\Gamma^T J) \bullet N^d \int_{Q_k^N} \varphi \, dx = \sum_{k \in \mathbb{Z}_N^d} J_k \bullet \int_{Q_k^N} \Gamma \varphi \, dx = \langle j, \Gamma \varphi \rangle.$$

In particular, for all $\varphi \in C^\infty(\mathbb{T}^d)$ we obtain $\langle \dot{c}, \iota_N^* \varphi \rangle_N = -\langle \overline{\text{div}} F, \iota_N^* \varphi \rangle_N + \langle \Gamma^* J, \iota_N^* \varphi \rangle_N$ if and only if $\langle \partial_t \iota_N c, \varphi \rangle = -\langle \text{div} f, \varphi \rangle + \langle \Gamma^* j, \varphi \rangle$.

This finishes the proof of Lemma 3.16. \square

4 Main results

Before we state our main results, we fix the assumptions on our problem.

Assumption 4.1 (General assumptions). *The continuous reference measure has a density $\omega \in C(\mathbb{T}^d, \mathbb{R}^I)$ and there exists ω_* , ω^* such that for all $x \in \mathbb{T}^d$, $i \in I$ it holds*

$$0 < \omega_* \leq \omega_i(x) \leq \omega^* < \infty. \quad (3.G1)$$

The diffusion and reaction coefficients satisfy

$$\forall r \in R: \quad \kappa_r > 0 \quad \text{and} \quad \forall i \in I: \quad \delta_i \geq \delta_* > 0. \quad (3.G2)$$

We emphasize that our analysis carries over without difficulty to diffusion and reaction coefficients that are non-constant in space, but are continuous and uniformly bounded above and away from zero.

For each $N \in \mathbb{N}$ we define the discrete reference measure $w^N = (w_i^N)_{i \in I} \in \mathcal{P}(X_N)$ by

$$w_{i,k}^N := \iota_N^* \omega_i = N^d \int_{Q_k^N} \omega_i \, dx.$$

We immediately observe that the bounds on the continuous reference measure translate uniformly to all discrete reference measures, i.e., for all $N \in \mathbb{N}$, $i \in I$, and $k \in \mathbb{Z}_N^d$ it holds

$$0 < \omega_* \leq w_{i,k}^N \leq \omega^* < \infty. \quad (4.1)$$

Moreover, we easily obtain the following convergences

$$\iota_N w^N \rightarrow \omega \text{ strongly in } L^\infty(X), \quad (4.2a)$$

$$\forall e \in E \forall i \in I: \quad S_e^N(\iota_N w_i^N) \rightarrow \omega_i \text{ strongly in } L^\infty(\mathbb{T}^d). \quad (4.2b)$$

The above natural Assumptions 4.1 as well as their simple consequence are used throughout the paper without always referring to them.

With this notation and under these general assumptions, we can formulate the energy-dissipation principle for the discrete system. Here we follow an idea in [PR*22, Thm. 4.16] and consider the function

$$B(c, v) = \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} b\left(\frac{c_{i,k}}{w_{i,k}^N}, v_{i,k}\right) \quad \text{with } b(a, s) = \begin{cases} s \log a & \text{for } a > 0, \\ 0 & \text{for } a = 0. \end{cases}$$

The special treatment of the singularity of $\log c_{i,k}$ at $c_{i,k}$ leads to nontrivial implications that can only be handled due to the property that the underlying (discrete) reaction-diffusion system preserves non-negativity or, even more, positivity.

Lemma 4.2 (Chain rule for the discrete setting). *Let $c \in AC([0, T]; L^1(X_N))$ be such that*

$$t \mapsto B(c(t), \dot{c}(t)) \text{ lies in } L^1(0, T).$$

Then, $t \mapsto E_N(c(t))$ is absolutely continuous and we have the chain rule formula

$$\frac{d}{dt} E_N(c(t)) = B(c(t), \dot{c}(t)) \text{ for a.a. } t \in [0, T]. \quad (4.3)$$

In particular, every curve $(c, F, J) \in \overline{CE}$ with $D_N(c, F, J) < \infty$ satisfies

$$E_N(c(t)) - E_N(c(s)) = \int_s^t B(c(r), \dot{c}(r)) \, dr \geq - \int_s^t (R_N(c(r), F(r), J(r)) + S_N(c(r))) \, dr.$$

This result will be a consequence of the more detailed Proposition 6.1. With this chain rule it is then possible to show that discrete EDB solutions are equivalent to ODE solutions, i.e., in the discrete setting the Energy-Dissipation Principle holds.

Theorem 4.3 (Discrete EDB and (1.3)). *A function $c \in AC([0, T]; \mathcal{M}_+(X_N))$ is a solution to the discrete reaction-diffusion system (1.3) if and only if the triple (c, F, J) with F and J given by (6.4) is a discrete EDB solution in the sense of Definition 3.8.*

We refer to the end of Section 6.1 for the proof.

We now turn to the continuum system, where we need to restrict the stoichiometric vectors α^r and β^r , which was not the case in the discrete setting. At the end of this section we will shortly address the case where we have a priori bounds in L^∞ , which is again a case, where arbitrary stoichiometric vectors are allowed.

In our analysis we will use two levels of assumptions: the first is needed for deriving the lower-limit estimates and the second, which is slightly stronger, will be used to derive the abstract chain rule.

Assumption 4.4 (for lower-limit estimates). *The reaction coefficients satisfy*

$$\forall r \in R : \frac{1}{2} |\alpha^r + \beta^r|_1 \leq p_{\text{crit}} := 1 + 2/d. \quad (4.A1)$$

Assumption 4.5 (for chain rule inequality). *The reaction coefficients satisfy*

$$\forall r \in R : |\alpha^r|_1 \leq p_{\text{crit}}, \quad |\beta^r|_1 \leq p_{\text{crit}}, \quad \frac{1}{2} |\alpha^r + \beta^r|_1 \leq p_{\text{crit}}. \quad (4.A2)$$

Example 4.6. *In all space dimensions we have $p_{\text{crit}} > 1$. Hence, our analysis covers linear exchange reactions*

$$X_1 \rightleftharpoons X_2 \quad \text{where } |\alpha|_1 = |\beta|_1 = \frac{1}{2} |\alpha + \beta|_1 = 1.$$

In space dimensions $d \leq 2$ we have $p_{\text{crit}} = 3$ or $p_{\text{crit}} = 2$, which allows to handle binary reactions with $j = c_1 c_2 - c_3$, i.e.,

$$X_1 + X_2 \rightleftharpoons X_3 \quad \text{where } |\alpha|_1 = 2, \quad |\beta|_1 = 1, \quad \frac{1}{2} |\alpha + \beta|_1 = 3/2,$$

or the semi-conductor reaction with $j = c_{\text{neg}} c_{\text{pos}} - 1$, i.e.,

$$X_{\text{neg}} + X_{\text{pos}} \rightleftharpoons \emptyset \quad \text{where } |\alpha|_1 = 2, \quad |\beta|_1 = 0, \quad \frac{1}{2} |\alpha + \beta|_1 = 1.$$

Having fixed the assumptions, we now state the convergence of the discrete gradient systems to the continuum gradient system.

Theorem 4.7 (Convergence and lower limit of energy-dissipation functionals). *Consider $(c^N, F^N, J^N) \in \overline{CE}_N$ such that the uniform bounds $\sup_{N \in \mathbb{N}} \text{ess sup}_{t \in [0, T]} E_N(c^N(t)) < \infty$ and $\sup_{N \in \mathbb{N}} D_N(c^N, F^N, J^N) < \infty$ hold true. Moreover, assume that the reactions satisfy (4.A1).*

Then, there exists $(\rho, f, j) \in CE$ with $f \in L^1([0, T] \times Y_{\text{diff}})$ and $j \in L^1([0, T] \times Y_{\text{react}})$ such that (up to a subsequence) we have $\iota_N c^N \rightarrow \rho$ strongly in $L^1([0, T] \times X)$, $\iota_{N, \text{diff}} F^N \rightharpoonup f$ weakly in $L([0, T] \times Y_{\text{diff}})$, and $\iota_{N, \text{react}} J^N \rightharpoonup j$ weakly in $L^1([0, T] \times Y_{\text{react}})$.

Moreover, we have the lower limit inequalities

$$\liminf_{N \rightarrow \infty} D_N(c^N, F^N, J^N) \geq \mathcal{D}(\rho, f, j) \quad \text{and} \quad \liminf_{N \rightarrow \infty} E_N(c^N(t)) \geq \mathcal{E}(\rho(t)) \quad \text{for all } t \in [0, T],$$

for the functionals defined in (3.1), (3.5), (3.7), and (3.8), respectively.

In particular, for well-prepared initial data, i.e., $\iota_N c^N(0) \rightarrow \rho(0)$ with $E_N(c^N(0)) \rightarrow \mathcal{E}(\rho(0))$, it holds

$$\liminf_{N \rightarrow \infty} L_N(c^N, F^N, J^N) \geq \mathcal{L}(\rho, f, j).$$

To conclude that the limit (ρ, f, j) solves the limit gradient-flow equation, we need in addition a chain rule inequality for the continuous reaction-diffusion system. (Recall \mathcal{D} and \mathcal{L} from Definition 3.11.)

Theorem 4.8 (Chain rule inequality for continuum system). *Consider a curve $(\rho, f, j) \in \text{CE}$ with $\mathcal{D}(\rho, f, j) < \infty$ and $\text{ess sup}_{t \in [0, T]} \mathcal{E}(\rho(t)) < \infty$. In addition, assume that the reaction coefficients satisfy (4.A2).*

Then, for every $0 \leq s < t \leq T$ it holds

$$\mathcal{E}(\rho(t)) - \mathcal{E}(\rho(s)) + \int_s^t \mathcal{R}(\rho(\tau), f(\tau), j(\tau)) + \mathcal{S}(\rho(\tau)) \, d\tau \geq 0.$$

Furthermore, it holds $\mathcal{L}(\rho, f, j) = 0$ if and only if ρ is a continuum EDB solution of (1.2) in the sense of Definition 3.13.

The three theorems together imply that solutions of the discrete problems (1.3) on \mathbb{Z}_N^d starting from well-prepared initial data converge (after choosing a suitable subsequence) to solutions of the continuous reaction-diffusion system (1.2). This is summarized in our final main result.

Corollary 4.9 (Convergence of solutions). *Assume that the reactions satisfy (4.A2). Let $\rho_0 \in L^1(X)$ satisfy $\mathcal{E}(\rho_0) < \infty$. Let $(c_0^N)_{N \in \mathbb{N}}$ with $c_0^N \in L^1(X_N)$ be well-prepared, i.e., let $\iota_N c_0^N \rightarrow \rho_0$ in $L^1(X)$ and $E_N(c_0^N) \rightarrow \mathcal{E}(\rho_0)$ as $N \rightarrow \infty$.*

Then, for each $N \in \mathbb{N}$ there exists a solution $c^N \in L^1(0, T; \mathcal{M}_+(X_N))$ of (1.3) on \mathbb{Z}_N^d in the sense of Definition 3.8 with initial datum c_0^N .

Furthermore, (up to a subsequence) we have $\iota_N c^N \rightarrow \rho$ strongly in $L^1([0, T] \times X)$, where ρ is a solution of the gradient flow equation (1.2) on \mathbb{T}^d in the sense of Definition 3.13 with initial datum ρ_0 .

The proofs of the main results are given in the next two sections: In Section 5, we show the necessary compactness and the lower limit of dissipation functionals leading to Theorem 4.7. In Section 6 we show that the chain rules and energy-dissipation principles for both, the discrete and the continuous, reaction-diffusion systems hold.

Finally, we comment on the restrictions on the stoichiometric vectors. In fact, they are needed for deriving suitable a priori bounds. If however, these bounds can be obtained by other means, then the conditions can be dropped completely.

Remark 4.10 (L^∞ bounds via bounding boxes). *It can be easily checked that the proofs given below hold for general stoichiometric vectors α^r and β^r , if we know that the discrete solutions c^N are bounded uniformly in L^∞ . Indeed, in this case the limit solution ρ is also bounded in L^∞ and we can set $p_{\text{crit}} = \infty$ and check that all proofs work similarly.*

We highlight this fact since for several classes of reaction-diffusion systems there exist so-called positively invariant regions in the sense of [Smo94, Cha. 14§B]. In the simplest case such a region is a rectangular set, also called bounding box:

$$\mathbb{B} := \prod_{i \in I} [0, b_i] := \{ c \in [0, \infty)^I \mid 0 \leq c_i \leq b_i \text{ for all } i \in I \}.$$

Positive invariance means that solutions starting inside a region (i.e. $c(t, x) \in \mathbb{B}$) remain inside the region for all $t > 0$. In the case of a box the invariance follows, if for $c \in \partial \mathbb{B}$ the reaction vector $R(c)$ points inwards, i.e., $c_i = 0$ implies $R_i(c) \geq 0$ and $c_i = b_i$ implies $R_i(c) \leq 0$.

Consider a reaction systems where all reactions are of the type $\alpha_i X_i \rightleftharpoons \beta_i X_i$ which is additionally in detailed balance for $w = (w_i)_{i \in I}$. Then, it can be shown that $\mathbb{B} = \prod_I [0, w_i]$ is indeed a bounding box. Often there is a family of detailed-balance equilibria w , which then allow for arbitrary large bounding boxes.

5 Proof of convergence

The aim of this section is to prove Theorem 4.7, the convergence of the discrete gradient systems to the continuum gradient system. We split the section in two parts, first focusing on the compactness in Section 5.1, before establishing the lower limit in Section 5.2.

To show compactness, we rely on the N -uniform L^∞ -bound for the energies and the N -uniform bound of the dissipation functionals to obtain suitable a priori estimates for the embedded discrete concentrations $\rho^N = \iota_N c^N$. We introduce a new and efficient method to show equi-integrability of the fluxes F^N and J^N in Proposition 5.5. Finally, an argument based on the Aubin-Lions-Simon lemma allows us to derive strong compactness of ρ^N in Proposition 5.8. One of the biggest advantages of our approach is its ability of handling non-convex dependencies on ρ^N of the dissipation functionals.

The lower limit inequalities are then obtained for each rate and each slope term, independently, relying either on Ioffe's liminf theorem or, for the diffusive rate, on a dualization argument.

Throughout this section, we fix a time horizon $T > 0$ and denote by $\Omega_T := [0, T] \times \mathbb{T}^d$ the parabolic cylinder.

5.1 Compactness

We start our considerations from the N -uniform L^∞ -bound on the energies and the N -uniform bound on the dissipations. We introduce the explicit constants K_x^A that will make it easier to see the influence of the different bounds throughout the section.

We start with the a priori bounds

$$K^E := \sup_{N \in \mathbb{N}} \sup_{t \in [0, T]} E_N(c^N(t)) < \infty, \quad (5.1a)$$

$$K^D := \sup_{N \in \mathbb{N}} D_N(c^N, F^N, J^N) < \infty. \quad (5.1b)$$

In particular, these imply

$$K_{L^1}^E := \sup_{N \in \mathbb{N}} \sup_{t \in [0, T]} \|c^N\|_{L^1_N} < \infty, \quad (5.2a)$$

$$K_{\text{diff}}^R := \sup_{N \in \mathbb{N}} \int_0^T R_{N, \text{diff}}(c^N(t), F^N(t)) dt < \infty, \quad (5.2b)$$

$$K_{\text{react}}^R := \sup_{N \in \mathbb{N}} \int_0^T R_{N, \text{react}}(c^N(t), J^N(t)) dt < \infty, \quad (5.2c)$$

$$K_{\text{diff}}^S := \sup_{N \in \mathbb{N}} \int_0^T S_{N, \text{diff}}(c^N(t)) dt < \infty, \quad (5.2d)$$

$$K_{\text{react}}^S := \sup_{N \in \mathbb{N}} \int_0^T S_{N, \text{react}}(c^N(t)) dt < \infty. \quad (5.2e)$$

Using the embeddings from Section 3.3, we define the curves

$$\rho^N := \iota_N c^N, \quad f^N := \iota_{N, \text{diff}} F^N, \quad j^N := \iota_{N, \text{react}} J^N.$$

To derive strong relative compactness of $(\rho^N)_{N \in \mathbb{N}}$ in $L^1([0, T] \times X)$, we rely on an Aubin-Lions-type result. Since these piecewise constant functions are not weakly differentiable and we will later rely on Sobolev embeddings to obtain higher integrability, we introduce a second interpolant $\tilde{\rho}^N$ via

$$\tilde{\rho}_i^N = \omega_i (\tilde{\iota}_N U_i^N)^2 \quad \text{where} \quad U_{i,k}^N = \left(\frac{c_{i,k}}{w_{i,k}^N} \right)^{1/2}, \quad (5.3)$$

where the linear interpolator $\tilde{\iota}_N$ generates continuous and piecewise polynomial functions $\tilde{u}^N = \tilde{\iota}_N U^N$, the derivatives of which can be controlled uniformly in N by K_{diff}^S .

Employing an Aubin-Lions-Simon-type argument, we show relative compactness of $(\tilde{\rho}^N)_{N \in \mathbb{N}}$. We then conclude by showing that $\|\tilde{\rho}^N - \rho^N\|_{L^1([0, T] \times X)} \rightarrow 0$ as $N \rightarrow \infty$.

We highlight that, we will be able to show that ρ^N is bounded in an Orlicz space slightly better than $L^{p_{\text{crit}}}([0, T] \times \mathbb{T}^d)$ with $p_{\text{crit}} = 1 + 2/d$.

Remark 5.1. Note that our particular choice for the auxiliary embedding \tilde{t}_N is the d -linear interpolation, though we stress that other interpolations are possible as long as Lemma 5.3 is provable. In particular, we believe it is possible to employ a similar argument for more general geometries when replacing the uniform grids \mathbb{Z}_N^d .

Furthermore, we point out that strong L^1 compactness of ρ^N could also be obtained directly by applying [RoS03, Theorem 4.2] as is done, e.g. in [HrT23, Theorem 4.8]. However, our method additionally allows us to obtain higher integrability as we demonstrate in Proposition 5.4.

Definition 5.2 (Continuous embedding). Let $M := \{0, 1\}^d$. For $m \in M$ we define the functions $f_m^N : \mathbb{T}^d \rightarrow [0, 1]$ via

$$f_m^N(x) = \prod_{k=1}^d \begin{cases} Nx_k & \text{for } m_k = 1 \\ 1 - Nx_k & \text{for } m_k = 0 \end{cases} \quad \text{for } x \in Q_0^N \quad \text{and} \quad f_m^N(x) = 0 \quad \text{otherwise.}$$

Recalling the shift operator S_y^N from (3.12), we define the continuous embedding operator

$$\tilde{t}_N(U_i^N)(x) := \tilde{u}_i^N(x) := \sum_{k \in \mathbb{Z}_N^d} \sum_{m \in M} U_{i,k+m}^N f_m^N(x - k/N) \quad (5.4)$$

and its dual discretization operator

$$\tilde{t}_N^*(\varphi_i)_k = N^d \int_{Q_k^N} \sum_{m \in M} S_{-m}^N \varphi_i(x) S_{-k}^N f_m^N(x) dx.$$

The duality of \tilde{t}_N and \tilde{t}_N^* follows by a direct calculation:

$$\begin{aligned} \int_{\mathbb{T}^d} \varphi_i \tilde{t}_N U_i^N dx &= \sum_{k \in \mathbb{Z}_N^d} \sum_{m \in M} U_{i,k+m}^N \int_{Q_k^N} \varphi_i(x) S_{-k}^N f_m^N(x) dx \\ &= \sum_{k \in \mathbb{Z}_N^d} \sum_{m \in M} U_{i,k}^N \int_{Q_{k-m}^N} \varphi_i(x) S_{-m}^N f_m^N(x) dx = \sum_{k \in \mathbb{Z}_N^d} \sum_{m \in M} U_{i,k}^N \int_{Q_k^N} S_{-m}^N \varphi_i(x) S_{-k}^N f_m^N(x) dx \\ &= \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} U_{i,k}^N N^d \int_{Q_k^N} \sum_{m \in M} S_{-m}^N \varphi_i(x) S_{-k}^N f_m^N(x) dx = \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \tilde{t}_N^*(\varphi_i)_k U_{i,k}^N. \end{aligned}$$

To understand the usage of the functions f_m^N better it is useful to define the functions

$$h_0^N(x) = \sum_{m \in M} S_m^N f_m^N(x) \quad \text{and} \quad h_k^N = S_{-k}^N h_0^N.$$

Then, all h_k^N are piecewise polynomial and *continuous*, and the simple interpolation formula

$$\tilde{u}_i^N = \tilde{t}_N U_i^N = \sum_{k \in \mathbb{Z}_N^d} U_{i,k}^N h_k^N$$

holds. The following properties of f_m^N and h_k^N will be used in the sequel without further specification:

$$f_m^N(x) \in [0, 1], \quad \int_{\mathbb{T}^d} f_m^N(x) dx = \frac{1}{(2N)^d}, \quad \sum_{m \in M} f_m^N(x) = \mathbb{1}_{Q_0^N}(x), \quad (5.5a)$$

$$h_m^N(x) \in [0, 1], \quad \int_{\mathbb{T}^d} h_k^N(x) dx = \frac{1}{N^d}, \quad \sum_{k \in \mathbb{Z}_N^d} h_k^N(x) = 1 \text{ on } \mathbb{T}^d, \quad (5.5b)$$

$$\|\nabla h_m^N\|_{L^\infty} \leq N, \quad \|\nabla h_m^N\|_{L^1} \leq C_d, \quad h_k^N(x) \geq \frac{1}{2^d} S_{\frac{1}{2}\mathbf{1}_d}^N \mathbb{1}_{Q_k^N}(x), \quad (5.5c)$$

where we denoted $\mathbf{1}_d = (1, \dots, 1) \in \mathbb{R}^d$. The next results shows that the concentrations c^N enjoy a higher integrability as the one obtained from the uniform bound K^E for E_N . For this we use the bound K_{diff}^S in (5.2d) and a suitable Galiardo-Nirenberg interpolation applied to \tilde{u}^N . We first show that $\nabla \tilde{u}^N$ is uniformly bounded in $L^2([0, T] \times \mathbb{T}^d)$, which is a consequence of the fact that $S_{N,\text{diff}}(c^N)$ is in fact a quadratic form in U^N .

Lemma 5.3 (Spatial regularity). *Let c^N satisfy the a priori estimates (5.2d). Then, we have*

$$\iint_{\Omega_T} |\nabla \tilde{u}^N|^2 dx dt \leq \left(\frac{4}{3}\right)^{d-1} \frac{K_{\text{diff}}^S}{\delta_* \omega_*}$$

Proof. We work for fixed N and i and hence drop these indices throughout this proof.

We recall that each h_k is nontrivial only on 2^d cubes Q_{k-m} . Moreover, fixing $l \in \{1, \dots, d\}$ the derivative $\partial_{x_l} h_k$ has positive values in those 2^{d-1} cubes with $m_l = 1$ and negative values in those with $m_l = 0$:

$$\partial_{x_l} h_k = \underbrace{\partial_{x_l} h_k \mathbb{1}_{V_{l,k}}}_{\geq 0} - \underbrace{\left(-\partial_{x_l} h_k \mathbb{1}_{V_{l,k+e_l}}\right)}_{\geq 0} \quad \text{with } V_{l,k} = \bigcup_{\substack{m \in M \\ m_l = 1}} Q_{k-m}^N.$$

Using $\partial_{x_l} h_k = -\partial_{x_l} h_{k-e_l}$ on $V_{l,k}$ we find

$$\partial_{x_l} \tilde{u} = \sum_{k \in \mathbb{Z}_N^d} U_k \partial_{x_l} h_k = \sum_{k \in \mathbb{Z}_N^d} (U_k - U_{k-e_l}) \partial_{x_l} h_k \mathbb{1}_{V_{l,k}}.$$

At each $x \in \mathbb{T}^d$ there are at most 2^{d-1} terms, since each $V_{l,k}$ consists of 2^{d-1} small cubes. Hence, we obtain

$$\int_{\mathbb{T}^d} |\partial_{x_l} \tilde{u}|^2 dx \leq 2^{d-1} \int_{\mathbb{T}^d} \sum_{k \in \mathbb{Z}_N^d} |U_k - U_{k-e_l}|^2 |\partial_{x_l} h_k|^2 \mathbb{1}_{V_{l,k}} dx = \left(\frac{4}{3}\right)^{d-1} \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} N^2 |U_k - U_{k-e_l}|^2,$$

where we used $\int_{\mathbb{T}^d} |\partial_{x_l} h_k|^2 \mathbb{1}_{V_{l,k}} dx = N^2 (2/3)^{d-1}$. This concludes the proof. \square

To obtain uniform higher integrability of the densities ρ^N we combine the spatial regularity with the uniform energy bound (5.1a). The former provides L^2 integrability in time in the good space $H^1(\mathbb{T}^d)$ while the latter provides boundedness of $\mathcal{E}(\tilde{\rho}^N)$ which is slightly better than $\text{ess sup } \tilde{\rho}^N(t) \leq K_{L^1}^E$. We will exploit the following interpolation estimate that follows by applying a suitable Gagliardo-Nirenberg interpolation, see Appendix C for the proof of a more general version. Setting $\alpha \geq 2$, $\alpha d \in [4, 4+2d]$ and $q = 2d/(4-(\alpha-2)d) \in [1, \infty]$, it holds the bilinear interpolation estimate

$$\iint_{\Omega_T} u^\alpha v dx dt \leq C \|v\|_{L^\infty(0,T;L^q(\mathbb{T}^d))} \|u\|_{L^\infty(0,T;L^2(\mathbb{T}^d))}^{\alpha-2} \int_0^T \|u(t)\|_{H^1(\mathbb{T}^d)}^2 dt, \quad (5.6)$$

for a suitable constant C depending on d and α . To estimate $\tilde{\rho}_i^N = \omega_i (\tilde{u}^N)^2$ we will apply this estimate for $u = \tilde{u}_i^N$ and either $v \equiv 1$ or $v = \lambda_B((\tilde{u}_i^N)^2)^\beta$.

Proposition 5.4 (Improved integrability). *Let c^N satisfy the a priori estimates (5.1a), (5.2a), and (5.2d). Then, with $p_{\text{crit}} = 1 + 2/d$ from Assumption (4.A1) we have*

$$\sup_{N \in \mathbb{N}} \|c^N\|_{L^{p_{\text{crit}}}([0,T] \times X_N)} \leq C_{(1)}, \quad (5.7a)$$

where $C_{(1)}$ only depends on d, ω_*, ω^* and δ_* . Moreover, with $\eta_d = 2/d$ for $d \geq 3$, $\eta_2 \in (0, 1)$, and $\eta_1 = 1$, there exists $C_{(2)} > 0$ depending on $d, \omega_*, \omega^*, \delta_*, K^E, K_{L^1}^E$ such that

$$\sup_{N \in \mathbb{N}} \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \sum_{i \in I} \int_0^T (c_{i,k}^N)^{p_{\text{crit}}} (\log(1 + c_{i,k}^N))^{\eta_d} dt \leq C_{(2)}. \quad (5.7b)$$

In particular, analogous N -uniform estimates to (5.7a) and (5.7b) also hold for ρ^N .

Proof. We consider only one species i and drop its index throughout this proof. In light of (5.5c), it is sufficient to prove the spatial regularity for $\tilde{\rho}^N$. From the definition of $\tilde{\rho}^N = \omega (\tilde{u}^N)^2$ we immediately obtain $\|\tilde{u}^N(t)\|_{L^2}^2 \leq K_{L^1}^E / \omega_*$. Applying (5.6) with $u = \tilde{u}_i^N$, $v \equiv 1$ and $\alpha = 2p_{\text{crit}}$ (which implies $q = \infty$), we find

$$\iint_{\Omega_T} (\tilde{u}^N)^{2p_{\text{crit}}} dx dt \leq C \|\tilde{u}^N\|_{L^\infty(0,T;L^2)}^{4/d} \int_0^T \|\tilde{u}^N\|_{H^1(X)}^2 dt.$$

Using $\tilde{\rho}^N = \omega(\tilde{u}^N)^2$ and Lemma 5.3, we obtain (5.7a).

For the second part we choose $u = \tilde{u}_i^N$ and $v = \lambda_B((\tilde{u}^N)^2)^{\eta_d}$. For $d \geq 3$ let $\alpha = 2$ and $q = d/2$ to find

$$\iint_{\Omega_T} u^2 \lambda_B(u^2)^{2/d} dx dt \leq \int_0^T \|u\|_{L^{2d/d-2}}^2 \|\lambda_B(u^2)\|_{L^1} dt \leq CK_E^{2/d} K_{\text{diff}}.$$

For $d = 1$ we choose $\alpha = 4$ and $q = 1$ giving

$$\iint_{\Omega_T} u^4 \lambda_B(u^2) dx dt \leq \int_0^T \|u\|_{L^\infty}^4 \|\lambda_B(u^2)\|_{L^1} dt \leq CK_E^2 K_{\text{diff}}^S.$$

For $d = 2$ we choose $\eta_2 \in (0, 1)$ arbitrary and set $q = 1/\eta_2$ and $\alpha = 4 - 2\eta_2$. This leads to the estimate

$$\begin{aligned} \iint_{\Omega_T} u^{4-2\eta_2} \lambda_B(u^2)^{\eta_2} dx dt &\leq \int_0^T \|u\|_{L^{(4-2\eta_2)/(1-\eta_2)}}^{4-2\eta_2} \|\lambda_B(u^2)\|_{L^{1/\eta_2}}^{1/\eta_2} dt \\ &= \int_0^T \|u\|_{L^{(4-2\eta_2)/(1-\eta_2)}}^{4-2\eta_2} \|\lambda_B(u^2)\|_{L^1} dt \leq C(\eta_2) K_E^2 K_{\text{diff}}, \end{aligned}$$

where $C(\eta_2) \rightarrow \infty$ for $\eta_2 \nearrow 1$.

Using $u^q \log(e+u)^\eta \leq C u^{q-2\eta} (1 + \lambda_B(u^2))^\eta$ and $\tilde{\rho}^N \leq \omega^*(\tilde{u}^N)^2$, the estimate (5.7b) follows. \square

The higher integrability derived in (5.7b) will allow us to show that the diffusion fluxes $f^N = \iota_{N,\text{diff}} F^N$ and the reaction fluxes $j^N = \iota_{N,\text{react}} J^N$ are uniformly equi-integrable, and hence one may choose a subsequence converging weakly in $L^1(\Omega_T)$. The estimate for f^N will rely on the magical estimate (3.4d), whereas the estimate for j^N has to be based on the weaker result of Lemma 3.3.

Proposition 5.5 (Boundedness of fluxes). *Assume (4.A1) and let (c^N, F^N, J^N) satisfy the a priori estimates (5.1). Then, there exist constants $C_{\text{flux}}^{\text{diff}} > 0$ and $C_{\text{flux}}^{\text{react}} > 0$ and a convex superlinear function $\Phi_d : \mathbb{R} \rightarrow [0, \infty)$ depending only on d , such that for all $N \in \mathbb{N}$, $e \in E$, $i \in I$, and $r \in R$ s we have*

$$\frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T \mathbb{C}\left(\frac{F_{i,k,e}^N}{N}\right) dt \leq C_{\text{flux}}^{\text{diff}} \quad \text{and} \quad \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T \Phi_d(J_{r,k}^N) dt \leq C_{\text{flux}}^{\text{react}},$$

where $C_{\text{flux}}^{\text{diff}}$ ($C_{\text{flux}}^{\text{react}}$) depends only on the constants $C_{(1)}$ and $C_{(2)}$ from (5.7) and K_{diff}^R (K_{react}^R).

Moreover, there exist curves of fluxes f and j with $f_{i,e} \in L^1(\Omega_T)$ and $j_r \in L^1(\Omega_T)$ such that along a (not renamed) subsequence, we have

$$\begin{aligned} \iint_{\Omega_T} \mathbb{C}(f_{i,e}) dx dt &\leq C_{\text{flux}}^{\text{diff}} \quad \text{and} \quad \iint_{\Omega_T} \Phi_d(j_r) dx dt \leq C_{\text{flux}}^{\text{react}}, \\ f_{i,e}^N &\rightharpoonup f_{i,e} \quad \text{and} \quad j_r^N \rightharpoonup j_r \quad \text{weakly in } L^1(\Omega_T), \end{aligned}$$

where we recall $f^N = \iota_{N,\text{diff}} F^N$ and $j^N = \iota_{N,\text{react}} J^N$ defined in (3.10a) and (3.10c), respectively.

Proof. We consider the diffusive flux $F_{i,e}^N$ first, where we fix and then omit the indices i, e . We apply the magical estimate (3.4d) with $q = p_{\text{crit}} > 1$ to obtain

$$\begin{aligned} \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T \mathbb{C}\left(\frac{1}{N} F_k^N\right) dt &\leq \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T \left(\frac{p_{\text{crit}}}{p_{\text{crit}}-1} \mathbb{C}\left(\frac{1}{N} F_k^N \mid \sigma_k^N\right) + \frac{4}{p_{\text{crit}}-1} (\sigma_k^N)^2 \right) dt \\ &\leq C_{p_{\text{crit}}} \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T \left(\mathbb{C}(F_k^N \mid N^2 \sigma_k^N) + (\sigma_k^N)^{p_{\text{crit}}} \right) dt \\ &\leq C_{p_{\text{crit}}} K_{\text{diff}}^R + C_{p_{\text{crit}}} \|\sigma^N\|_{L^{p_{\text{crit}}}([0,T] \times \mathbb{Z}_N^d)}^{p_{\text{crit}}}, \end{aligned}$$

where the estimate from the second to the third line follows from the monotonicity (3.4c) and where we used that $\sigma_{i,e}^N = \delta_i(c_{i,k} c_{i,k+e})^{1/2}$ is uniformly bounded in $L^{p_{\text{crit}}}$ by $C_{(1)}$ in (5.7a).

The argument for j_r^N is analogous, however, we have to be aware that we now have to choose $\sigma_r^N = \kappa_r (c^N)^{\gamma^r}$ with $\gamma^r = \frac{1}{2}(\alpha^r + \beta^r)$. Thus, (5.7a) and assumption (4.A1) only provide a uniform bound for σ_r^N in L^1 . However, Lemma 3.3 can be employed on the basis of the improved higher regularity. We choose $\phi = C$ and

$$\psi_d(w) = w \left(\log(1+w^{1/p_{\text{crit}}}) \right)^{1/d},$$

which is increasing and superlinear. Thus, the function $\Xi_d = \Xi_{C, \psi_d}$ is still superlinear and increasing, and the same is true for its convex hull $\Phi_d = (\Xi_d)^{**} \leq \Xi_d$. With this, fixing and omitting the index r , we can estimate

$$\begin{aligned} \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T \Phi_d(J_k^N) dt &\leq \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T \Xi_d(J_k^N) dt \leq \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T (\mathfrak{C}(J_k^N | \sigma_k^N) + \psi_d(\sigma_k^N)) dt \\ &\leq K_{\text{flux}}^{\text{react}} + \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T |c^N|^{p_{\text{crit}}} (\log(1+|c_k^N|))^{1/d} dt \leq K_{\text{flux}}^{\text{react}} + C_{(2)} \end{aligned}$$

with $C_{(2)}$ from (5.7b).

For the embedded diffusive fluxes $f^N = \iota_{N, \text{diff}} F^N$, we recall that (3.10b) involves a partition of unity. Therefore, it follows $\iint_{\Omega_T} C(f^N) dx dt \leq \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T C(\frac{1}{N} F_k^N) dt$ by an application of Jensen's inequality. Similarly, we have for the embedded reactive fluxes the estimate $\iint_{\Omega_T} \Phi_d(j^N) dx dt \leq \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \int_0^T \Phi_d(J_k^N) dt$.

With this, the criterion of de la Vallée Poussin shows that the sequences $(f^N)_N$ and $(j^N)_N$ both are sequentially compact in the weak topology of $L^1(\Omega_T)$. Thus, a subsequence (not relabeled) and limits f and j exist such that $f^N \rightharpoonup f$ and $j^N \rightharpoonup j$. Moreover, the convexity of C and Φ_d implies the weak lower semi-continuities $\int_{\Omega_T} C(f_{i,e}) dx dt \leq \liminf_{N \rightarrow \infty} \int_{\Omega_T} C(f_{i,e}^N) dx dt \leq C_{\text{flux}}^{\text{diff}}$ and $\int_{\Omega_T} \Phi_d(j_r) dx dt \leq \liminf_{N \rightarrow \infty} \int_{\Omega_T} \Phi_d(j_r^N) dx dt \leq C_{\text{flux}}^{\text{react}}$.

With this, the proof of Proposition 5.5 is complete. \square

Remark 5.6. The uniform equi-integrability for the diffusive rate $\iint C(F_{i,e}^N) dx dt \leq C_{\text{flux}}^{\text{diff}}$ was also obtained in [HrT23, Lem. 4.4] by a slightly different and more generally applicable argument that only uses that σ^N is uniformly bounded in $L^\infty(0, T; L^1(\mathbb{T}^d))$.

Having established the spatial regularity of $\tilde{\rho}^N$ in Lemma 5.3 as well as boundedness of the fluxes in Proposition 5.5, our next step is to show time regularity for $\tilde{\rho}^N$.

Lemma 5.7 (Time regularity). *Assume (4.A1) and let (c^N, F^N, J^N) satisfy the a priori estimates (5.1). Then, we have the uniform bound $\sup_{N \in \mathbb{N}} \|\tilde{\rho}^N\|_{BV(0, T; (W^{1, \infty}(X))^*)} < \infty$.*

Proof. We first focus on the more complicated interpolation $\tilde{\iota}_N$ and recall (3.13), which implies for every $\varphi \in C^1(X)$

$$\begin{aligned} \langle F^N, \nabla \tilde{\iota}_N^* \varphi \rangle &= \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} \sum_{i \in I} F_{i,k,e}^N [(\tilde{\iota}_N^* \varphi)_{i,k+e} - (\tilde{\iota}_N^* \varphi)_{i,k}] \\ &= \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} \sum_{i \in I} \sum_{m \in M} F_{i,k,e}^N \int_{Q_k^N} S_{-k}^N f_m^N S_{-m}^N [S_e^N \varphi_i - \varphi_i] dx \\ &= \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} \sum_{i \in I} \sum_{m \in M} \frac{F_{i,k,e}^N}{N} \int_{Q_k^N} \int_0^1 S_{-k}^N f_m^N(x) S_{\theta-m}^N \partial_{x_e} \varphi_i(x) d\theta dx \\ &\leq C_M \|\nabla \varphi\|_{L^\infty(X)} \sum_{i \in I} \sum_{e \in E} \left\| \frac{F_{i,e}^N}{N} \right\|_1. \end{aligned}$$

Similarly, for every $\varphi \in C(X)$ we have

$$\begin{aligned} \langle J^N, \Gamma \tilde{\iota}_N^* \varphi \rangle &= \sum_{k \in \mathbb{Z}_N^d} \sum_{r \in R} J_{r,k}^N \sum_{i \in I} \gamma_{r,i} \sum_{m \in M} \int_{Q_k^N} S_{-k}^N f_m^N S_{-m}^N \varphi_i dx \\ &\leq \|\varphi\|_{L^\infty(X)} \max_{s \in R} \sum_{i \in I} |\gamma_{s,i}| \sum_{r \in R} \|J_r^N\|_1. \end{aligned}$$

With this, we consider any partition $(t_m)_{m=0}^M$, $M \in \mathbb{N}$ of $[0, T]$. Then, the previous bounds, the discrete continuity equation, and Proposition 5.5 yield, for every $\varphi \in C^1(X)$, the estimate

$$\begin{aligned} \sum_{m=1}^M \langle \tilde{\rho}^N(t_m) - \tilde{\rho}^N(t_{m-1}), \varphi \rangle &= \sum_{m=1}^M \langle c^N(t_m) - c^N(t_{m-1}), \tilde{\iota}_N^* \varphi \rangle_N \\ &= \sum_{m=1}^M \int_{t_{m-1}}^{t_m} \langle F^N, \nabla \tilde{\iota}_N^* \varphi \rangle + \langle J^N, \Gamma \tilde{\iota}_N^* \varphi \rangle dt \leq C \|\varphi\|_{C^1(X)}. \end{aligned}$$

Taking suprema with respect to $\varphi \in \{\varphi \in C^1(X) : \|\varphi\|_{W^{1,\infty}(X)} \leq 1\}$ and the partition, we obtain the uniform bound $\sup_N \|\tilde{\rho}^N\|_{\text{BV}(0,T;(W^{1,\infty})^*)} < \infty$. This finishes the proof of Lemma 5.7. \square

Combining the spatial regularity of \tilde{u} from Lemma 5.3 and the time regularity of $\tilde{\rho}$ from Lemma 5.7, we are now able to apply the Aubin-Lions-Simon lemma to obtain strong L^1 compactness for $\tilde{\rho}^N$. We then show that ρ^N has the same strong limit by comparing it to $\tilde{\rho}^N$.

Proposition 5.8 (Strong compactness). *Assume (4.A1) and let (c^N, F^N, J^N) satisfy the a priori estimates (5.1).*

Then, there exists $\rho \in L^{\text{pcrit}}([0, T] \times X)$ such that along a (not renamed) subsequence both $\tilde{\rho}^N \rightarrow \rho$ strongly in $L^1([0, T] \times X)$ and $\rho^N \rightarrow \rho$ strongly in $L^1([0, T] \times X)$.

Furthermore, it holds $\rho \in \text{AC}([0, T]; \mathcal{M}_+(X))$ and $\rho^N(t) \rightharpoonup^ \rho(t)$ weakly-* in $\mathcal{M}_+(X)$ for all $t \in [0, T]$.*

Proof. Lemma 5.3 implies that $\tilde{\rho}^N \in L^1([0, T]; Z)$, where $Z := \{\omega u^2 : u \in H^1(X)\}$. Since $\omega \in L^\infty(X)$, we have the compact embedding $Z \Subset L^1(X)$. Combining this with Lemma 5.7, we obtain the existence of $\rho \in L^1([0, T] \times X)$ such that $\tilde{\rho}^N \rightarrow \rho$ strongly in $L^1([0, T] \times X)$ by applying the Aubin-Lions-Simon Lemma, [Sim86, Theorem 5].

For the convergence of ρ^N , we compare it to $\tilde{\rho}^N$ and recall that $U_k^N = \sqrt{\frac{c_k^N}{w_k^N}}$ to derive

$$\begin{aligned} \|\tilde{\rho}^N - \rho^N\|_{L^1([0,T] \times X)} &= \left\| \omega \left(\tilde{\iota}_N \sqrt{\frac{c^N}{w^N}} \right)^2 - \iota_N c^N \right\|_{L^1([0,T] \times X)} \\ &\leq \omega^* \left\| \left(\tilde{\iota}_N \sqrt{\frac{c^N}{w^N}} \right)^2 - \iota_N \frac{c^N}{w^N} \right\|_{L^1([0,T] \times X)} + \left\| \omega \iota_N \frac{c^N}{w^N} - \iota_N c^N \right\|_{L^1([0,T] \times X)} \\ &\leq \omega^* \left\| (\tilde{\iota}_N U_k^N)^2 - \iota_N (U_k^N)^2 \right\|_{L^1([0,T] \times X)} + \frac{K_{L^1}^E}{\omega_*} \|\omega - \iota_N w^N\|_{L^\infty([0,T] \times X)}. \end{aligned}$$

The second summand on the right-hand side vanishes as $N \rightarrow \infty$ by (4.2a). To control the first summand, we first employ (5.5) to obtain for all $x \in \mathbb{T}^d$ the auxiliary inequality

$$\begin{aligned} \left(\sum_{k \in \mathbb{Z}_N^d} (h_k^N \pm \mathbb{1}_{Q_k^N}) U_k^N \right)^2 &= \sum_{k,l \in \mathbb{Z}_N^d} \sum_{m,n \in M} (S_{m-k}^N f_m^N(x) \pm S_{-k}^N f_m^N(x)) (S_{n-l}^N f_n^N(x) \pm S_{-l}^N f_n^N(x)) U_k^N U_l^N \\ &= \sum_{k,l \in \mathbb{Z}_N^d} \sum_{m,n \in M} S_{-k}^N f_m^N(x) S_{-l}^N f_n^N(x) (U_{k+m}^N \pm U_k^N) (U_{l+n}^N \pm U_l^N) \\ &= \sum_{k \in \mathbb{Z}_N^d} \sum_{m,n \in M} S_{-k}^N f_m^N(x) S_{-k}^N f_n^N(x) (U_{k+m}^N \pm U_k^N) (U_{k+n}^N \pm U_k^N) \\ &\leq 2^d \sum_{k \in \mathbb{Z}_N^d} \sum_{m,n \in M} \mathbb{1}_{Q_k^N}(x) (U_{k+m}^N \pm U_k^N) (U_{k+n}^N \pm U_k^N) \\ &\leq 2^d \sum_{k \in \mathbb{Z}_N^d} \sum_{m \in M} \mathbb{1}_{Q_k^N}(x) |U_{k+m}^N \pm U_k^N|^2. \end{aligned}$$

We combine this with Hölder's inequality to find

$$\left\| (\tilde{\iota}_N U_k^N)^2 - \iota_N (U_k^N)^2 \right\|_{L^1([0,T] \times X)} = \left\| \left(\sum_{k \in \mathbb{Z}_N^d} h_k^N U_k^N \right)^2 - \sum_{k \in \mathbb{Z}_N^d} \mathbb{1}_{Q_k^N} (U_k^N)^2 \right\|_{L^1([0,T] \times X)}$$

$$\begin{aligned}
&= \left\| \left(\sum_{k \in \mathbb{Z}_N^d} h_k^N U_k^N \right)^2 - \left(\sum_{k \in \mathbb{Z}_N^d} \mathbb{1}_{Q_k^N} U_k^N \right)^2 \right\|_{L^1([0, T] \times X)} \\
&\leq \left\| \sum_{k \in \mathbb{Z}_N^d} (h_k^N + \mathbb{1}_{Q_k^N}) U_k^N \right\|_{L^2([0, T] \times X)}^{\frac{1}{2}} \left\| \sum_{k \in \mathbb{Z}_N^d} (h_k^N - \mathbb{1}_{Q_k^N}) U_k^N \right\|_{L^2([0, T] \times X)}^{\frac{1}{2}} \\
&\leq 2^d \left\| \sum_{m \in M} (U_{k+m}^N + U_k^N) \right\|_{L^2([0, T] \times X_N)}^{\frac{1}{2}} \left\| \sum_{m \in M} (U_{k+m}^N - U_k^N) \right\|_{L^2([0, T] \times X_N)}^{\frac{1}{2}} \\
&\leq C_M \sqrt{\frac{K_{L^1}^E K_{\text{diff}}^s K_{\text{diff}}^S}{\omega_*} \frac{1}{\delta_* \omega_* N}},
\end{aligned}$$

where in the last step we used that each $m \in M$ is a sum of finitely many d -dimensional unit vectors, estimated the first factor using (5.1a), and extracted the power $1/N$ from the second factor by estimating with the uniform bound (5.2d) and Definition 3.4.

Moreover, by Proposition 5.4 the curves ρ^N are N -uniformly bounded in $L^{\text{pcrit}}([0, T] \times X)$, so is the limit ρ . This concludes the proof of Proposition 5.8.

The weak-* convergence $\rho^N(t) \rightharpoonup^* \rho(t)$ for all $t \in [0, T]$ follows from the bounds in Proposition 5.5 by arguing analogously to [HrT23, Lemma 4.5].

□

To later obtain a lower limit inequality for the dissipation functionals, we must ensure that the limit objects from Proposition 5.5 and Proposition 5.8 satisfy the continuity equation. This fact is established in the following lemma:

Lemma 5.9 (Closedness of CE). *Let (ρ, j, f) be a limit of $(\rho^N, j^N, f^N)_{N \in \mathbb{N}} \subset \text{CE}$ in the sense of Propositions 5.8 and 5.5. Then, it holds $(\rho, j, f) \in \text{CE}$.*

Proof. By definition the set CE is closed with respect to the weak- L^1 convergence of the time-integrated embedded fluxes shown in Proposition 5.5 and the pointwise-in-time weak-* convergence of the embedded concentrations shown in Proposition 5.8. □

To prove the lower limit inequality for the slopes, we will employ a convergence result for the differences of the piecewise constantly embedded concentrations. This is established next.

Proposition 5.10 (Convergence of differences). *Assume (4.A1) and let (c^N, F^N, J^N) satisfy the a priori estimates (5.1). Let ρ be the limit of $(\iota_N c^N)_N$ from Proposition 5.8. Recalling $U_{i,k}^N = (c_{i,k}/w_{i,k}^N)^{1/2}$, we introduce $u_i^N = \iota_N U_{i,k}^N$, $u := ((\rho_i/\omega_i)^{1/2})_i$, and $\nabla_N u^N := \frac{1}{N} \sum_{e \in \mathbb{E}} (S_e^N u^N - u^N)e$.*

Then, it holds $u \in L^2(0, T; H^1(\mathbb{T}^d))$, $u^N \rightarrow u$ strongly in $L^2([0, T] \times X)$ and along a (not renamed) subsequence $\nabla_N u^N \rightharpoonup \nabla u$ weakly in $L^2([0, T] \times X)$.

Proof. Throughout this proof we fix an arbitrary species i and omit the corresponding index. We denote $\omega^N = \iota_N w^N$. The strong L^2 convergence $u^N \rightarrow u$ immediately follows by integrating the estimate

$$|u^N - u|^2 = \left| \sqrt{\frac{\rho^N}{\omega^N}} - \sqrt{\frac{\rho}{\omega}} \right|^2 \leq \left| \frac{\rho^N}{\omega^N} - \frac{\rho}{\omega} \right| \leq \frac{1}{\omega_*} |\rho^N - \rho| + \frac{1}{\omega_*^2} |\rho| |\omega^N - \omega|,$$

and using Assumption 4.1.

Next, we consider the differences $\nabla_N u^N = \frac{1}{N} \sum_{e \in \mathbb{E}} (S_e^N u^N - u^N)e$. Since ι_N commutes with multiplication, it holds $\|\nabla_N u^N\|_{L^2(\Omega_T; \mathbb{R}^d)}^2 \leq \delta \omega^* K_{\text{diff}}^S$ and hence (along a not renamed subsequence) $\nabla_N u^N \rightharpoonup v$ weakly in $L^2(\Omega_T; \mathbb{R}^d)$ for some $v \in L^2(\Omega_T; \mathbb{R}^d)$. This v is the weak gradient of u . Indeed, let $\varphi \in C^\infty(\Omega_T)$. Then, for every $e \in \mathbb{E}$ (and the

above subsequence) we have

$$\begin{aligned} \iint_{\Omega_T} v(t, x) \cdot e \varphi(t, x) \, dx \, dt &= \lim_{N \rightarrow \infty} \iint_{\Omega_T} \left(\frac{u^N(t, x + e/N) - u^N(t, x)}{1/N} \right) \varphi(t, x) \, dx \, dt \\ &= \lim_{N \rightarrow \infty} \iint_{\Omega_T} u^N(t, x) \left(\frac{\varphi(t, x - e/N) - \varphi(t, x)}{1/N} \right) \, dx \, dt \\ &= - \iint_{\Omega_T} u(t, x) \partial_{x_e} \varphi(t, x) \, dx \, dt. \end{aligned}$$

In particular, $u \in L^2([0, T]; H^1(\mathbb{T}^d))$ and the proof is concluded. \square

5.2 Lower limit of dissipation functionals

In the previous section we have obtained candidate curves that may be EDB solutions for (1.2). Following the strategy of Section 2.2, the next step is to prove rigorous analogs of (2.4). More precisely, we will prove lower limit inequalities for the rate and slope terms independently. First, we consider the slopes, employing a Ioffe's liminf theorem.

Proposition 5.11. *Assume (4.A1) and let (c^N, F^N, J^N) satisfy the a priori estimates (5.1). Let $u_i = \sqrt{\rho_i/\omega_i}$ be the L^2 -limit of $u_i^N = \iota_N \sqrt{c_i^N w_i^N}$ from Proposition 5.10. Then, it holds*

$$\liminf_{N \rightarrow \infty} \int_0^T S_N(c^N) \, dt \geq \int_0^T \mathcal{S}(\rho) \, dt$$

Proof. By Proposition 5.10 we have along a (not renamed) subsequence $\nabla_N u_i^N \rightharpoonup \nabla u_i$ weakly in $L^2(\Omega_T; \mathbb{R}^d)$. Thus, an application of Ioffe's liminf theorem, [But89, Thm. 2.3.1], directly yields the lower limit for the diffusive part:

$$\liminf_{N \rightarrow \infty} \int_0^T S_{N,\text{diff}}(c^N) \, dt \geq \sum_{i \in I} 2\delta_i \int_0^T \int_{\mathbb{T}^d} |\nabla u_i|^2 \, d\omega_i \, dt = \int_0^T \mathcal{S}_{\text{diff}}(\rho) \, dt.$$

For the reactive part, by definition of ι_N , we have

$$\begin{aligned} S_{N,\text{react}}(c^N) &= \sum_{r \in R} 2\kappa_r \frac{1}{N^d} \sum_{k \in \mathbb{Z}_N^d} (w_k^N)^{(\alpha^r + \beta^r)/2} \left| \left(\frac{c_k^N}{w_k^N} \right)^{\alpha^r/2} - \left(\frac{c_k^N}{w_k^N} \right)^{\beta^r/2} \right|^2 \\ &= \sum_{r \in R} 2\kappa_r \int_{\mathbb{T}^d} (\omega^N)^{(\alpha^r + \beta^r)/2} \left| (u^N)^{\alpha^r} - (u^N)^{\beta^r} \right|^2. \end{aligned}$$

On the other hand, it holds $(u^N)^\lambda(t, x) \rightarrow u^\lambda(t, x)$ and $w^N(x) \rightarrow \omega(x)$ for \mathcal{L} -a.e. $t \in [0, T]$ and \mathcal{L}^d -a.e. $x \in \mathbb{T}^d$, and every multiindex $\lambda \in \mathbb{R}^I$. Thus, Fatou's Lemma with $f_N = (\omega^N)^{(\alpha^r + \beta^r)/2} \left| (u^N)^{\alpha^r} - (u^N)^{\beta^r} \right|^2$ yields

$$\liminf_{N \rightarrow \infty} \int_0^T S_{N,\text{react}}(c^N) \, dt \geq \sum_{r \in R} 2\kappa_r \int_0^T \int_{\mathbb{T}^d} \omega^{(\alpha^r + \beta^r)/2} \left| u^{\alpha^r} - u^{\beta^r} \right|^2 \, dt = \int_0^T \mathcal{S}_{\text{react}}(\rho) \, dt,$$

which concludes the proof. \square

Next, we focus on the rate parts of the dissipation potentials. Here, the main challenge is the diffusive rate, where we want to obtain the quadratic dissipation from the cosh-type dissipation. The proof is done by dualization following the proof of [HrT23, Thm. 6.2 (i)]. First, we link the cosh-type and quadratic dual dissipation potentials in the following lemma.

Lemma 5.12. *Let $(c^N)_{N \in \mathbb{N}}$ be any sequence s.t. $\iota_N c^N =: \rho^N \rightharpoonup \rho$ in $L^1(X)$. Moreover, let $\varphi \in C^1(X)$ be given. Then, it holds*

$$\limsup_{N \rightarrow \infty} R_{N,\text{diff}}^*(c^N, \bar{\nabla} \iota_N^* \varphi) \leq \mathcal{R}_{\text{diff}}^*(\rho, \nabla \varphi).$$

In particular, we have for $\iota_N c^N \rightarrow \rho$ in $L^1([0, T] \times X)$ and any $\varphi \in L^1(0, T; C^1(X))$ that

$$\limsup_{N \rightarrow \infty} \int_0^T R_{N,\text{diff}}^*(c^N(t), \bar{\nabla} \iota_N^* \varphi(t)) \, dt \leq \int_0^T \mathcal{R}_{\text{diff}}^*(\rho(t), \nabla \varphi(t)) \, dt.$$

Proof. For $\varphi \in C^1(X)$, we have

$$\begin{aligned} |\iota_N^* \varphi_{i,k+e} - \iota_N^* \varphi_{i,k}| &\leq N^d \int_{\mathbb{T}^d} |\varphi_i(x) (\mathbb{1}_{Q_{k+e}^N}(x) - \mathbb{1}_{Q_k^N}(x))| dx \\ &= N^d \int_{Q_k^N} |\varphi_i(x) - \varphi_i(x + e/N)| dx \\ &\leq N^d \int_{Q_k^N} |\partial_{x_e} \varphi_i(x)| \cdot |e/N| dx = \frac{1}{N} \iota_N^* (|\partial_{x_e} \varphi_i|)_k. \end{aligned}$$

Using that $C^*(r) = C^*(-r) = C^*(|r|)$ and the monotonicity of $[0, \infty) \ni r \mapsto C^*(r)$, we compute

$$\begin{aligned} R_{N,\text{diff}}^*(c^N, \bar{\nabla} \iota_N^* \varphi) &= \frac{1}{N^d} \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in \mathbb{E}} N^2 \delta_i(c_{i,k}^N c_{i,k+e}^N)^{1/2} C^*(\iota_N^* \varphi_{i,k+e} - \iota_N^* \varphi_{i,k}) \\ &= \frac{1}{N^d} \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in \mathbb{E}} N^2 \delta_i(c_{i,k}^N c_{i,k+e}^N)^{1/2} C^*(|\iota_N^* \varphi_{i,k+e} - \iota_N^* \varphi_{i,k}|) \\ &\leq \frac{1}{N^d} \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in \mathbb{E}} N^2 \delta_i(c_{i,k}^N c_{i,k+e}^N)^{1/2} C^*\left(\frac{1}{N} \iota_N^* (|\partial_{x_e} \varphi_i|)_k\right). \end{aligned}$$

Note that, by the definition of C^* , for all $r \in [0, \infty)$ and all $N \in \mathbb{N}$ it holds

$$N^2 C^*\left(\frac{r}{N}\right) \leq \frac{r^2}{2} \cosh\left(\frac{r}{N}\right).$$

Our aim is to apply this with $r = \iota_N^* (|\partial_{x_e} \varphi_i|)_k$, which is why we introduce the scalar

$$a_N := \max_{k \in \mathbb{Z}_N^d, i \in I, e \in \mathbb{E}^d} \left\{ \cosh\left(\frac{1}{N} \iota_N^* (|\partial_{x_e} \varphi_i|)_k\right) \right\} \in [1, \infty),$$

and observe that $a_N \rightarrow 1$ as $N \rightarrow \infty$. Then, we can conclude that

$$\begin{aligned} R_{N,\text{diff}}^*(c^N, \bar{\nabla} \iota_N^* \varphi) &\leq a_N \frac{1}{N^d} \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in \mathbb{E}} \delta_i(c_{i,k}^N c_{i,k+e}^N)^{1/2} \frac{1}{2} (\iota_N^* (|\partial_{x_e} \varphi_i|)_k)^2 \\ &\leq a_N \frac{1}{N^d} \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in \mathbb{E}} \delta_i \frac{c_{i,k}^N + c_{i,k+e}^N}{2} \frac{1}{2} (\iota_N^* (|\partial_{x_e} \varphi_i|)_k)^2 \\ &\leq a_N \frac{1}{N^d} \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in \mathbb{E}} \delta_i \frac{c_{i,k}^N + c_{i,k+e}^N}{2} \frac{1}{2} \iota_N^* (|\partial_{x_e} \varphi_i|_k^2) \\ &= a_N \sum_{i \in I} \sum_{e \in \mathbb{E}} \delta_i \langle (c_i^N + S_e^N c_i^N)/2, \frac{1}{2} \iota_N^* (|\partial_{x_e} \varphi_i|^2) \rangle_N \\ &= a_N \sum_{i \in I} \delta_i \left\langle \iota_N (c_i^N + S_e^N c_i^N)/2, \sum_{e \in \mathbb{E}} \frac{1}{2} |\partial_{x_e} \varphi_i|^2 \right\rangle \\ &= a_N \sum_{i \in I} \delta_i \langle \iota_N (c_i^N + S_e^N c_i^N)/2, |\nabla \varphi_i|^2/2 \rangle \\ &\xrightarrow{N \rightarrow \infty} \mathcal{R}_{\text{diff}}^*(\rho, \nabla \varphi), \end{aligned}$$

where we have used that for all $\psi \in C(\mathbb{T}^d)$ it holds

$$\langle \iota_N S_e^N c_i^N, \psi \rangle = \sum_{k \in \mathbb{Z}_N^d} \int_{Q_k^N} c_{i,k+e} \psi(x) dx = \sum_{k \in \mathbb{Z}_N^d} \int_{Q_k^N} c_{i,k} \psi(x - e/N) dx \xrightarrow{N \rightarrow \infty} \langle \rho_i, \psi \rangle.$$

This proves the first claim. The second claim follows by Fatou's lemma and the pointwise convergence of the integral. \square

Having linked the cosh-type and quadratic dual dissipation potentials, we are now in the position to obtain the lower limit for the diffusive rates using duality arguments. For the reactive rate part there is no change in the structure, thus allowing us to again employ Ioffe's liminf theorem.

Proposition 5.13. *Assume (4.A1) and let (c^N, F^N, J^N) satisfy the a priori estimates (5.1). Moreover, let ρ be the limit from $\iota_N c^N$ from Proposition 5.8, and let f and j be the limits of $\iota_{N,\text{diff}} F^N$ and $\iota_{N,\text{react}} J^N$ from Proposition 5.5, respectively. Then, we have*

$$\liminf_{N \rightarrow \infty} \int_0^T R_N(c^N, F^N, J^N) dt \geq \int_0^T \mathcal{R}(\rho, f, j) dt.$$

Proof. First, we consider the reactive part. Observe that we have

$$R_{N,\text{react}}(c, J) = \mathcal{R}_{\text{react}}(\iota_N c^N, \iota_N J^N).$$

Hence, the estimate for the reactive parts follows from Ioffe's liminf theorem, [But89, Thm. 2.3.1], for the convex function $J \mapsto \mathcal{C}(J|_{\kappa_r}(c^{\alpha^r} c^{\beta^r})^{1/2})$ from the weak-L¹ convergence of J^N and the strong-L¹ convergence of $(\rho^N)^{\frac{1}{2}(\alpha^r + \beta^r)}$ by (4.A1).

For the diffusive part, we employ the Lemma 5.12. By the duality of \mathbb{C} and \mathbb{C}^* , we have

$$\begin{aligned} \langle F^N, \bar{\nabla} \iota_N^* \varphi \rangle_N &= \frac{1}{N^d} \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} (\bar{\nabla} \iota_N^* \varphi)_i)_{k,e} F_{i,k,e}^N \\ &\leq \frac{1}{N^d} \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} \sum_{e \in E} [N^2 \delta_i(c_{i,k}^N c_{i,k+e}^N)^{1/2} \mathbb{C}^*((\bar{\nabla} \iota_N^* \varphi)_i)_{k,e}) + \mathbb{C}(F_{i,k,e}^N | N^2 \delta_i(c_{i,k}^N c_{i,k+e}^N)^{1/2})] \\ &= R_{N,\text{diff}}^*(c^N, \bar{\nabla} \iota_N^* \varphi) + R_{N,\text{diff}}(c^N, F^N). \end{aligned}$$

Using $\varphi \in C^1([0, T] \times X)$, $\iota_N c^N dx = \rho^N \rightharpoonup^* \rho$, and $\iota_N F^N \rightharpoonup^* f$ and Lemma 5.12, we get

$$\begin{aligned} \int_0^T \langle f, \nabla \varphi \rangle - \mathcal{R}_{\text{diff}}^*(\rho, \nabla \varphi) dt &\leq \liminf_{N \rightarrow \infty} \int_0^T \langle F^N, \bar{\nabla} \iota_N^* \varphi \rangle_N dt - \limsup_{N \rightarrow \infty} \int_0^T R_{N,\text{diff}}^*(c^N, \bar{\nabla} \iota_N^* \varphi) dt \\ &\leq \liminf_{N \rightarrow \infty} \int_0^T \langle F^N, \bar{\nabla} \iota_N^* \varphi \rangle_N - R_{N,\text{diff}}^*(c^N, \bar{\nabla} \iota_N^* \varphi) dt \\ &\leq \liminf_{N \rightarrow \infty} \int_0^T R_{N,\text{diff}}(c^N, F^N) dt. \end{aligned}$$

The left-hand side is a quadratic functional in $\bar{\nabla} \varphi$ and hence can be continuously extended to its L^2 -closure $V := \{\bar{\nabla} \varphi : \varphi \in C^1([0, T] \times X)\}^{\text{L}^2(0, T; \text{L}^2_\rho(X^{\text{dom}}; Y_{\text{diff}}^{\text{tar}}))}$. Taking the supremum in V , we obtain $\int_0^T \mathcal{R}_{\text{diff}}(\rho, f) dt$ by duality. This finishes the proof. \square

Finally, we are in the position to prove Theorem 4.7.

Proof of Theorem 4.7. The asserted liminf inequality for dissipations follows from Proposition 5.11 and 5.13 together with the compactness results Proposition 5.5, Proposition 5.8, Lemma 5.9 and Proposition 5.10.

Regarding the liminf inequality for energies, we note that by definition of ι_N we have $E_N(c^N) = \mathcal{E}(\rho^N)$. Therefore, as \mathcal{E} is convex, the liminf inequality follows from the pointwise-in-time weak-* convergence of $\rho^N(t) \rightharpoonup^* \rho$ established in Proposition 5.8. \square

6 Proof of chain rules

In this section we prove the two chain rules stated above in Lemma 4.2 and Theorem 4.8 as well as the discrete and the continuum versions of the Energy-Dissipation principles of Theorem 4.3 and Proposition 3.14, respectively.

6.1 Chain rule for discrete reaction-diffusion system

We provide a full proof of the detailed chain rule in the discrete setting. A similar approach is given in [PR*22] for the case of linear reactions, i.e., where α^r, β^r are Euclidean unit vectors.

Recall from Section 4 the modification $B(c, \dot{c})$ of the duality product $DE_N(c) \cdot \dot{c}$, given by

$$B(c, v) = \sum_{i \in I} \sum_{k \in \mathbb{Z}_N^d} b\left(\frac{c_{i,k}}{w_{i,k}^N}, v_{i,k}\right) \quad \text{with } b(a, s) = \begin{cases} s \log a & \text{for } a > 0, \\ 0 & \text{for } a = 0. \end{cases}$$

The special treatment of the singularity of $\log c_{i,k}$ at $c_{i,k}$ leads to nontrivial implications that can only be handled due to the property that the underlying (discrete) reaction-diffusion system preserves non-negativity or even more positivity. For the linear scalar diffusion equation $u = \Delta u$ in our torus, it is well-known that $u(t_*, x_*) = 0$ for some $t_* > 0$ implies $u(t, x) = 0$ for all $t > 0$ and $x \in \mathbb{T}^d$. A similar statement holds for the discretization on \mathbb{Z}^d . However, for our reaction-diffusion system the situation is more complex, since some components are may vanish (identically) while other are positive. The gradient structure induced by the detailed-balance condition will provides enough control to handle the arising degeneracies.

Proposition 6.1 (Chain rule for the discrete setting).

a) Consider $c \in \text{AC}([0, T]; X_N)$ such that

$$t \mapsto B(c(t), \dot{c}(t)) \text{ lies in } L^1([0, T]).$$

Then, $t \mapsto E_N(c(t))$ is absolutely continuous and we have the chain rule formula

$$\frac{d}{dt} E_N(c(t)) = B(c(t), \dot{c}(t)) \text{ for a.a. } t \in [0, T]. \quad (6.1)$$

b) Consider a fixed vector (c, F, J) such that $c_{i,k} = 0$ implies $(\overline{\mathbb{G}}^*(F, J))_{i,k} = 0$, then

$$|B(c, \overline{\mathbb{G}}^*(F, J))| \leq R_N(c, F, J) + S_N(c) = R_{N,\text{diff}}(c, F) + R_{N,\text{react}}(c, J) + S_{N,\text{diff}}(c) + S_{N,\text{react}}(c). \quad (6.2)$$

c) We have the equality

$$B(c, \overline{\mathbb{G}}^*(F, J)) = R_N(c, F, J) + S_N(c) \quad (6.3)$$

if and only if

$$F_{i,k,e} = -\delta_i N^2 \sqrt{w_{i,k}^N w_{i,k+e}^N} \left(\frac{c_{i,k}}{w_{i,k}^N} - \frac{c_{i,k+e}}{w_{i,k+e}^N} \right) \quad \text{and} \quad J_{r,k} = \kappa_r (w_k^N)^{(\alpha_r + \beta_r)/2} \left(\frac{c_k^{\alpha_r}}{(w_k^N)^{\alpha_r}} - \frac{c_k^{\beta_r}}{(w_k^N)^{\beta_r}} \right). \quad (6.4)$$

In particular, (6.3) is equivalent to (1.3).

Proof. Without loss of generality, we may assume $w_{i,k}^N = 1$. Moreover, we may simplify the notation by only considering reactions, since for fixed N the jumps of c_i from k to $k+e$ are simple exchange reactions with reaction factor $\delta_i N^2$. (Formally, one can define $I' = I \times \mathbb{Z}_N^d$ and $R' = R \times \mathbb{Z}_N^d \cup I \times E \times \mathbb{Z}_N^d$.) Thus, in the rest of the proof, we omit the occurrence of N and $k \in \mathbb{Z}^d$, writing $c(t) \in [0, \infty)^I$ and $\overline{\mathbb{G}} = \Gamma$.

Part a). It suffices to consider only one species c_i and omit the index i , since E and B are both independent sums over i .

From $c \in \text{AC}([0, T]) = W^{1,1}([0, T])$ we have $c(t) \in [0, L]$ for some $L > 0$. For $c \geq 0$ and $\varepsilon \in (0, 1)$ we define $\beta_\varepsilon(c) = \max\{\log \varepsilon, \log c\}$ with $\beta_\varepsilon(0) = \log \varepsilon$ and $E_\varepsilon(c) = \int_1^c \beta_\varepsilon(s) ds$. With $\beta(c) = \log c$ for $c > 0$ and $\beta(0) = -\infty$ we have

$$\forall c \geq 0: \quad |\beta_\varepsilon(c)| \leq |\beta(c)| \quad \text{and} \quad 0 \leq E_\varepsilon(c) \nearrow E(c) \text{ as } \varepsilon \searrow 0.$$

Since E_ε is locally Lipschitz the chain rule holds: for $0 \leq s < t \leq T$ we have

$$E_\varepsilon(c(t)) - E_\varepsilon(c(s)) = \int_s^t b_\varepsilon(c(r), \dot{c}(r)) dr \quad \text{with } b_\varepsilon(c, v) = \beta_\varepsilon(c)v. \quad (6.5)$$

We claim that $|b_\varepsilon(c(r), \dot{c}(r))| \leq |b(c(r), \dot{c}(r))|$ a.e. in $[0, T]$, namely on the set where $\dot{c}(r)$ exists. For $c(r) > 0$ this follows immediately from $|\beta_\varepsilon(c)| \leq |\log(c)|$. If $c(r) = 0$ and $\dot{c}(r)$ exists, then $c(t) \geq 0$ for all $t \in [0, T]$ implies $\dot{c}(r) = 0$; and hence $b_\varepsilon(c(r), \dot{c}(r)) = 0 = b(c(r), \dot{c}(r))$.

By assumption $r \mapsto |b(c(r), \dot{c}(r))|$ is an integrable majorant for the integrand in (6.5). Moreover, we for a.a. r the convergence $b_\varepsilon(c(r), \dot{c}(r)) \rightarrow b(c(r), \dot{c}(r))$. Hence, we are able to pass to the limit $\varepsilon \rightarrow 0$ in (6.5), and the chain rule formula (6.1) follows.

Part b). Estimate (6.2) follows from the duality of R_N and R_N^* in the case $c_i \geq \delta > 0$, since $DE_N(c)$ is well defined and $S_N(c) = R_N^*(c, -\Gamma DE_N(c))$.

For the general case we introduce $c^\varepsilon = (c_i + \varepsilon)_{i \in I}$ for which (6.2) holds. We can pass to the limit $\varepsilon \searrow 0$ by noting the convergences on the right-hand side, as R_N and S_N are continuous in c (for fixed (F, J)), and on the left-hand side as well. For the latter we use the continuity of $c \mapsto \log c$ if $c_i > 0$ and $(\Gamma^* J)_i = 0$ if $c_i = 0$.

Part c). The case $c_i \geq \delta > 0$ is trivial since (6.2) implies

$$DE_N(c) \cdot \Gamma^* J \leq R_N(c, J) + R_N^*(c, -\Gamma DE_N(c)).$$

By strict convexity of $R_N(c, \cdot)$ we have equality if and only if $J = -D_\xi R_N^*(c, -\Gamma DE_N(c))$. Using (3.2a) we find the desired relation in (6.4).

For the general case, fix a vector (c, J) . We decompose the sets I and R into vanishing and positive parts:

$$I_v := \{i \in I \mid c_i = 0\}, \quad I_p := I \setminus I_v, \quad R_v := \{r \in R \mid \exists i \in I_v : \alpha_i^r + \beta_i^r > 0\}, \quad R_p := R \setminus R_v.$$

The equality (6.3) implies that the right-hand side must be finite. As $R_N(c, J)$ contains the terms $\mathbb{C}(J_r \mid \kappa_r c^{(\alpha^r + \beta^r)/2})$ and $c^{(\alpha^r + \beta^r)/2} = 0$ for all $r \in R_v$, we conclude $J_r = 0$ for all $r \in R_v$.

Rearranging the index sets I and R , we can write the $c = (c_p, c_v)$ and $J = (J_p, J_v)$ with $c_v = 0$ and $J_v = 0$. Writing $D_p E(c_p) = ((\log c_i)_{i \in I_p}, (0)_{i \in I_v})$, the desired equality (6.3) reduces to

$$\Gamma D_p E_N(c_p) \cdot (J_p, 0) = R_{N,p}(c_p, (J_p, 0)) + S_N(c_p, 0), \quad (6.6)$$

where $R_{N,p}$ is defined as R_N up to reducing the sum to $r \in R_p$, which implies that c_v does not appear any more. Since S is the sum over all reactions we have

$$S_N(c_p, 0) \geq S_{N,p}(c_p) := \sum_{r \in R_p} 2\kappa_r (c^{\alpha^r/2} - c^{\beta^r/2})^2 = R_{N,p}^*(c_p, -\Gamma D_p E_N(c_p)).$$

Replacing S_N by $S_{N,p}$, the convex duality of R_N and R_N^* implies

$$(J_p, 0) = -D_\xi R_{N,p}^*(c_p, -\Gamma D_p E_N(c_p)).$$

Moreover, the equality in (6.6) holds if and only if

$$S_N(c_p, 0) - S_{N,p}(c_p) = \sum_{r \in R_v} 2\kappa_r (c^{\alpha^r/2} - c^{\beta^r/2})^2 = 0.$$

Thus, we find $c^{\alpha^r} = 0 = c^{\beta^r}$ for all $r \in R_v$ (since at least one is 0 by definition and the difference vanishes by the last relation). Therefore, (6.4) holds true also in the general case. \square

Proposition 6.1 is exactly what we need to show that EDB solutions in the sense of Definition 3.8 are ODE solutions of the discrete system (1.3), which will complete the proof of the discrete Energy-Dissipation Principle.

Proof of Theorem 4.3. The direction from (1.3) to a EDB solution is classical, as the map $t \mapsto c(t)$ is $C^1([0, T]; \mathcal{M}(X_N))$.

For the opposite direction, we first observe that $L_N(c, F, J) = 0$ implies $D_N(c, F, J) < \infty$. By (6.2) we see that $t \mapsto B(c(t), \dot{c}(t))$ lies in $L^1([0, T])$. Hence, the chain rule (6.1) holds. Thus, we have

$$0 = L_N(c, F, J) = \int_0^T (B(c, \dot{c}) + R_N(c, F, J) + S_N(c)) dt.$$

Using $(c, F, J) \in \overline{CE}_N$ and (6.2), the integrand is non-negative, hence we conclude that the integrand has to vanish a.e. in $[0, T]$. Thus, F and J are given by the formulas in (6.4). Inserting this into the discrete continuity equation $\dot{c} + \overline{\mathbb{G}}^*(F, J) = 0$ gives exactly the desired ODE (1.3). \square

6.2 Chain rule for reaction-diffusion system on the torus

Before we prove Theorem 4.8, we first collect and prove two lemmas that we need in the following. First, we have the following inequality for the perspective function \mathbb{C} .

Lemma 6.2. *Let $\sigma > 0$. Then we have*

$$\forall j \in \mathbb{R} \forall a, b \geq \sigma : \quad |\mathbb{C}(j|a) - \mathbb{C}(j|b)| \leq \frac{2|j|}{\sigma} |a-b|. \quad (6.7)$$

Proof. We observe that $\partial_a \mathbb{C}(j|a) = m(j/a)$ with $m(r) = \mathbb{C}(r) - r\mathbb{C}'(r) = 4 - 2\sqrt{4+r^2} \leq 0$. Then, using $|m(r)| \leq 2|r|$ and $\mathbb{C}(j|b) - \mathbb{C}(j|a) = \int_a^b m(j/y) dy$, the result follows. \square

The lemma now helps to bound the difference once we have a bound on ρ and $j \in L^C([0, T] \times Y_{\text{react}})$. For this we recall the Hardy-Littlewood maximal function (see e.g. [Ste93]) which for a given function $g : \mathbb{R}^d \rightarrow \mathbb{R}$ is defined by

$$Mg(x) = \sup_{B \ni x} \frac{1}{|B|} \int_B |g(y)| dy,$$

where $B \subset \mathbb{R}^d$ are balls including x . It follows that $\sup_{\varepsilon > 0} |g * k_\varepsilon(x)| \leq Mg(x)$ for any measurable g . Regarding integration, there are classical results, showing that for $1 < p \leq \infty$ it holds $Mg \in L^p$ if $g \in L^p$. In the limiting case $p = 1$, one has the weaker statement $j \in L \log L$ (i.e. $\int_{\Omega_T} \mathbb{C}(|j|) dx dt < \infty$) if and only if $Mj \in L^1$, see [Ste69].

In the following proposition we will combine Lemma 6.2 with the estimate through the maximal function. For this, we need the magical estimate (3.4d), where the assumption $\frac{1}{2}|\alpha^r + \beta^r|_1 \lesssim p_{\text{crit}}$ is crucial to obtain $\rho^{(\alpha^r + \beta^r)/2} \in L^q(\Omega_T)$ with $q \gtrsim 1$. Unfortunately, a superlinear estimate for $|\rho|^{p_{\text{crit}}}$ as obtained in Proposition 5.4 would not be enough as is shown by the counterexample in Remark A.2.

The following result can also be seen as a commutator estimate, since it is essential to estimate $(\rho * k_\varepsilon)^{(\alpha^r + \beta^r)/2}$ against $(\rho^{(\alpha^r + \beta^r)/2}) * k_\varepsilon$, where k_ε is a smoothing kernel.

Proposition 6.3 (Commutator estimate). *Assume $\frac{1}{2}|\alpha^r + \beta^r|_1 \lesssim p$. Consider $\rho \in L^p([0, T] \times \mathbb{T}^d)$ and assume $\rho_i \geq \sigma > 0$ a.e. in Ω_T for all $i \in I$ and $\iint_{\Omega_T} \mathbb{C}(j_r |\rho^{(\alpha^r + \beta^r)/2}) dx dt < \infty$. Let k_ε be a mollifier approximating the identity, and $j_r^\varepsilon := j_r * k_\varepsilon$, $\rho^\varepsilon := \rho * k_\varepsilon$. Then, we have*

$$\limsup_{\varepsilon \rightarrow 0} \iint_{\Omega_T} \mathbb{C}(j_r^\varepsilon | (\rho^\varepsilon)^{(\alpha^r + \beta^r)/2}) dx dt \leq \iint_{\Omega_T} \mathbb{C}(j_r | \rho^{(\alpha^r + \beta^r)/2}) dx dt. \quad (6.8)$$

Proof. We drop the fixed index r for j_r , α_r , and β_r for the remainder of the proof and use the short-hand notations

$$\gamma := \frac{1}{2}(\alpha + \beta), \quad a := \rho^\gamma, \quad a_\varepsilon := (\rho^\varepsilon)^\gamma.$$

Using $|\gamma|_1 \lesssim p$ we have $a \in L^q(\Omega_T)$ with $q = p/|\gamma|_1 > 1$. Thus, we can use the magical property (3.4d) of \mathbb{C} and find

$$\iint_{\Omega_T} \mathbb{C}(j) dx dt \leq \iint_{\Omega_T} \left(\frac{q}{q-1} \mathbb{C}(j|a) + \frac{4}{q-1} a^q \right) dx dt < \infty.$$

This implies $j \in L \log L(\Omega_T)$, such that its Hardy-Littlewood maximal function (done in the space-time domain Ω_T) is integrable, i.e., $Mj \in L^1([0, T] \times Y_{\text{react}})$, see [Ste69]. Thus, we find the pointwise estimate

$$\forall \varepsilon > 0 : \quad |j_\varepsilon(t, x)| \leq Mj(t, x) \quad \text{almost everywhere in } \Omega_T, \quad (6.9)$$

this means that the family $(j_\varepsilon)_\varepsilon$ has a L^1 majorant.

Using the shorthand $x \wedge y = \min\{x, y\}$ for $x, y \in \mathbb{R}$, the monotonicity of $a \mapsto \mathbb{C}(s|a)$, and the bound (6.7) for the derivative in Lemma 6.2, we find for any $M > 0$ that

$$\begin{aligned} \mathbb{C}(j_\varepsilon | a_\varepsilon) &\leq \mathbb{C}(j_\varepsilon | M \wedge a_\varepsilon) \leq \mathbb{C}(j_\varepsilon | M \wedge b_\varepsilon) + g_\varepsilon \\ \text{with } g_\varepsilon &= \frac{2}{\sigma^{|\gamma|_1}} |j_\varepsilon| |(M \wedge b_\varepsilon) - (M \wedge a_\varepsilon)| \quad \text{and } b_{\varepsilon, M} = (a \wedge M) * k_\varepsilon. \end{aligned} \quad (6.10)$$

Using $b_{\varepsilon, M} \rightarrow a \wedge M$ and $a_\varepsilon \wedge M \rightarrow a \wedge M$ strongly in $L^q(\Omega_T)$ and weakly-* in $L^\infty(\Omega_T)$ as $\varepsilon \rightarrow 0$ together with (6.9), Lebesgue's dominated convergence theorem gives $G_\varepsilon = \iint_{\Omega_T} |g_\varepsilon| dx dt \rightarrow 0$.

Using $j_\varepsilon = j * k_\varepsilon$, $b_\varepsilon = a * k_\varepsilon$ and the joint convexity of $(j, a) \mapsto \mathbb{C}(j|a)$ allows us to apply Jensen's inequality. Hence, integrating the estimate (6.10) over Ω_T we find

$$\begin{aligned} \iint_{\Omega_T} \mathbb{C}(j_\varepsilon|a_\varepsilon) dx dt &\leq \iint_{\Omega_T} \mathbb{C}(j_\varepsilon|a_\varepsilon \wedge M) dx dt \leq \iint_{\Omega_T} (\mathbb{C}(j_\varepsilon|b_{\varepsilon, M}) + g_\varepsilon) dx dt \\ &\stackrel{\text{Jensen}}{\leq} \iint_{\Omega_T} \mathbb{C}(j|a \wedge M) dx dt + G_\varepsilon. \end{aligned}$$

Keeping M fixed and taking the upper limit $\varepsilon \rightarrow 0$ we find

$$\forall M \geq 1 : \limsup_{\varepsilon \rightarrow 0} \iint_{\Omega_T} \mathbb{C}(j_\varepsilon|a_\varepsilon) dx dt \leq \iint_{\Omega_T} \mathbb{C}(j|a \wedge M) dx dt.$$

To perform the limit $M \rightarrow \infty$, we use $\mathbb{C}(j|a \wedge M) \leq \mathbb{C}(j|a \wedge 1) \leq \max\{\mathbb{C}(j|1), \mathbb{C}(j|\rho^\gamma)\} \in L^1(\Omega_T)$ due to the assumption and $\mathbb{C}(j|1) = \mathbb{C}(j) \in L^1(\Omega_T)$. Hence, by dominated convergence the limit $M \rightarrow \infty$ provides the desired estimate (6.8). \square

Remark 6.4 (Convexity instead of commutator estimate). *The above commutator estimate can be avoided if the function $(\rho, s) \mapsto \mathbb{C}(s|\rho^\gamma)$ is jointly convex. Then, the result follows simply by applying Jensen's inequality for convolutions, i.e., $\iint \mathbb{C}(J * k_\varepsilon | (\rho * k_\varepsilon)^\gamma) dx dt \leq \iint \mathbb{C}(j|\rho^\gamma) dx dt$. This argument is usually used for linear reactions, see e.g. [Ste21, PR*22, Hrt23].*

Indeed, the joint convexity holds if and only if $|\gamma|_1 \leq 1$. Since $\mathbb{C}(s|g(\rho))$ is the Legendre-Fenchel transform of $g(\rho)\mathbb{C}^(\zeta)$, we have joint convexity if and only if $\rho \mapsto g(\rho)$ is concave. For $g(\rho) = \rho^\gamma$ the second derivative D^2g has the explicit form*

$$D^2g(\rho) = -\rho^\gamma \text{diag}(1/\rho_i)_I A(\gamma) \text{diag}(1/\rho_i)_I \quad \text{with } A(\gamma) = \text{diag}(\gamma) - \gamma \otimes \gamma.$$

Hence, g is concave if and only if $A(\gamma)$ is positive semi-definite. However, we have

$$b \cdot A(\gamma)b = \sum_{i \in I} \gamma_i b_i^2 - \left(\sum_{i \in I} \gamma_i b_i \right)^2 \geq \sum_{i \in I} \gamma_i b_i^2 - \left(\sum_{\bar{i} \in I} \gamma_{\bar{i}} \right) \left(\sum_{i \in I} \gamma_i b_i \right) = \left(1 - \sum_{\bar{i} \in I} \gamma_{\bar{i}} \right) \sum_{i \in I} \gamma_i b_i^2.$$

Hence, $\sum_{\bar{i} \in I} \gamma_{\bar{i}} \leq 1$ implies the desired concavity. However, considering the function $t \rightarrow g(tc) = t^\lambda c^\gamma$ gives $\lambda = \sum_{\bar{i} \in I} \gamma_{\bar{i}}$, and concavity implies $\lambda \leq 1$.

Putting the above results together, we can now prove Theorem 4.8.

Proof of Theorem 4.8. The proof is performed in several steps. First, we regularize and shift the density by a positive constant and show the chain rule for that situation. Then follows the harder part of estimating the limits. For this we rely on Proposition 6.3.

1. Step (Regularization): We note that from the bound on the energy and dissipation, the curve $t \mapsto \rho(t)$ is absolutely continuous with values in $(W^{1,\infty}(X))^*$ and it has a Lebesgue density ρdx for almost all $t \in [0, T]$. Furthermore, we have $\rho \in L^{p_{\text{crit}}}([0, T] \times X)$, $f \in L^1(0, T, Y_{\text{diff}})$, $j \in L^1([0, T] \times Y_{\text{react}})$ by Proposition 5.8 and Proposition 5.5. Given $\sigma > 0$ and a mollifier $(k_\varepsilon)_{\varepsilon > 0}$, we define the component-wise shifted and regularized trajectory

$$\rho^{\varepsilon, \sigma} := (\rho + \sigma) * k_\varepsilon,$$

and correspondingly the regularized fluxes $f^\varepsilon := f * k_\varepsilon$ and $j^\varepsilon := j * k_\varepsilon$. Clearly, $(\rho^{\varepsilon, \sigma}, f^\varepsilon, j^\varepsilon) \in \text{CE}$, where we have used that for the reactions the stoichiometric matrix Γ^* commutes with the mollification. Moreover, we have

$$\rho^{\varepsilon, \sigma} \rightarrow \rho \text{ in } L^1([0, T] \times X), \quad j^\varepsilon \rightarrow j \text{ in } L^1([0, T] \times Y_{\text{diff}}), \quad f^\varepsilon \rightarrow f \text{ in } L^1([0, T] \times Y_{\text{react}}).$$

2. Step (Chain rule for regularized curve): Now, we show that for fixed $\varepsilon, \sigma > 0$ the trajectory $t \mapsto \mathcal{E}(\rho^{\varepsilon, \sigma}(t))$ is absolutely continuous and satisfies the upper chain rule. For this, we first note that there is a constant $M_\varepsilon > 0$ such that $\|\rho^{\varepsilon, \sigma}\|_{L^\infty([0, T] \times \mathbb{T}^d)} \leq M_\varepsilon$ and we have $\rho^{\varepsilon, \sigma} \geq \sigma > 0$. To show absolute continuity, we fix $s, t \in [0, T]$, and since on

$[\sigma, M_\varepsilon + \sigma]$ the Boltzmann function $[\sigma, M_\varepsilon + \sigma] \ni r \mapsto \lambda_B(r) \in [0, \infty)$ is Lipschitz continuous, i.e., there is $L_{\sigma, \varepsilon} > 0$ such that $\forall r_1, r_2 \in [\sigma, M_\varepsilon + \sigma] : |\lambda'_B(r_1) - \lambda'_B(r_2)| \leq L_{\sigma, \varepsilon} |r_1 - r_2|$, we compute

$$\begin{aligned} \mathcal{E}(\rho^{\varepsilon, \sigma}(t)) - \mathcal{E}(\rho^{\varepsilon, \sigma}(s)) &\leq \sum_{i \in I} \int_{\mathbb{T}^d} |\lambda_B(\rho_i^{\varepsilon, \sigma}(t)) - \lambda_B(\rho_i^{\varepsilon, \sigma}(s))| dx \\ &\leq L_{\sigma, \varepsilon} \sum_{i \in I} \int_{\mathbb{T}^d} |\rho_i^{\varepsilon, \sigma}(t) - \rho_i^{\varepsilon, \sigma}(s)| dx = L_{\sigma, \varepsilon} \sum_{i \in I} \int_{\mathbb{T}^d} |\rho_i^\varepsilon(t) - \rho_i^\varepsilon(s)| dx. \end{aligned}$$

The mollifier k_ε is a test function in C_c^∞ with a (possibly bad) Lipschitz constant C_ε , which implies

$$\mathcal{E}(\rho^{\varepsilon, \sigma}(t)) - \mathcal{E}(\rho^{\varepsilon, \sigma}(s)) \leq C_\varepsilon L_{\sigma, \varepsilon} \|\rho(t) - \rho(s)\|_{(W^{1, \infty})^*}.$$

Hence, $t \mapsto \mathcal{E}(\rho^{\varepsilon, \sigma})$ is absolutely continuous, and we obtain by the differentiability of $r \mapsto \lambda_B(r)$ on $[\sigma, M_\varepsilon + \sigma]$ that

$$\begin{aligned} \frac{d}{dt} \mathcal{E}(\rho^{\varepsilon, \sigma}(t)) &= \sum_{i \in I} \int_{\mathbb{T}^d} \log(\rho_i^{\varepsilon, \sigma}(t)/\omega_i) \partial_t \rho_i^{\varepsilon, \sigma}(t) dx = \langle \log(\rho^{\varepsilon, \sigma}(t)/\omega), (-\operatorname{div} f^\varepsilon(t) + \Gamma^* j^\varepsilon(t)) \rangle \\ &= \langle \nabla \log(\rho^{\varepsilon, \sigma}(t)/\omega), f^\varepsilon(t) \rangle + \langle \Gamma \log(\rho^{\varepsilon, \sigma}(t)/\omega), j^\varepsilon(t) \rangle, \end{aligned}$$

which by integrating in time leads to

$$\mathcal{E}(\rho^{\varepsilon, \sigma}(t)) - \mathcal{E}(\rho^{\varepsilon, \sigma}(s)) = \int_s^t \langle \nabla \log(\rho^{\varepsilon, \sigma}(r)/\omega), f^\varepsilon(r) \rangle + \langle \Gamma \log(\rho^{\varepsilon, \sigma}(r)/\omega), j^\varepsilon(r) \rangle dr.$$

Here, we have used the chain rule with the nice test function $\nabla \log(\rho^{\varepsilon, \sigma}(r)/\omega)$. In particular, by Legendre duality we obtain

$$\begin{aligned} \mathcal{E}(\rho^{\varepsilon, \sigma}(t)) - \mathcal{E}(\rho^{\varepsilon, \sigma}(s)) &= - \int_s^t \langle \nabla \log(\rho^{\varepsilon, \sigma}(r)/\omega), -f^\varepsilon(r) \rangle + \langle \Gamma \log(\rho^{\varepsilon, \sigma}(r)/\omega), -j^\varepsilon(r) \rangle dr \\ &\geq - \int_s^t \mathcal{R}_{\text{diff}}(\rho^{\varepsilon, \sigma}, f^\varepsilon) + \mathcal{S}_{\text{diff}}(\rho^{\varepsilon, \sigma}) + \mathcal{R}_{\text{react}}(\rho^{\varepsilon, \sigma}, j^\varepsilon) + \mathcal{S}_{\text{react}}(\rho^{\varepsilon, \sigma}) dr. \end{aligned}$$

Hence, it follows the chain rule inequality for the regularized curve that $\mathcal{L}^{[s, t]}(\rho^{\varepsilon, \sigma}, f^\varepsilon, j^\varepsilon) \geq 0$.

3. Step (Limit $\sigma \rightarrow 0$ and $\varepsilon \rightarrow 0$): First, we observe that convergence of the energies is clear due to the convexity. Hence, it suffices to show that

$$\begin{aligned} \limsup_{\sigma \rightarrow 0} \limsup_{\varepsilon \rightarrow 0} \int_s^t \mathcal{R}_{\text{diff}}(\rho^{\varepsilon, \sigma}, f^\varepsilon) d\tau &\leq \int_s^t \mathcal{R}_{\text{diff}}(\rho, f) d\tau, \\ \limsup_{\sigma \rightarrow 0} \limsup_{\varepsilon \rightarrow 0} \int_s^t \mathcal{S}_{\text{diff}}(\rho^{\varepsilon, \sigma}) d\tau &\leq \int_s^t \mathcal{S}_{\text{diff}}(\rho) d\tau, \\ \limsup_{\sigma \rightarrow 0} \limsup_{\varepsilon \rightarrow 0} \int_s^t \mathcal{R}_{\text{react}}(\rho^{\varepsilon, \sigma}, j^\varepsilon) d\tau &\leq \int_s^t \mathcal{R}_{\text{react}}(\rho, j) d\tau, \\ \limsup_{\sigma \rightarrow 0} \limsup_{\varepsilon \rightarrow 0} \int_s^t \mathcal{S}_{\text{react}}(\rho^{\varepsilon, \sigma}) d\tau &\leq \int_s^t \mathcal{S}_{\text{react}}(\rho) d\tau. \end{aligned}$$

We will treat all four estimates and also the convergences $\sigma \rightarrow 0$ and $\varepsilon \rightarrow 0$ separately. In each term we will consider the limit $\varepsilon \rightarrow 0$ first, sending $\sigma \rightarrow 0$ afterwards.

3a (Diffusive terms): The rate term $\mathcal{R}_{\text{diff}}$ as well as the slope term $\mathcal{S}_{\text{diff}}$ are convex functionals. Hence, the upper limit bound for $\varepsilon \rightarrow 0$ follows by Jensen's inequality (see e.g. [AGS08, Lem. 8.1.10]) together with $\nabla \rho_i^\varepsilon \rightharpoonup \nabla \rho_i$, $j_r^\varepsilon \rightharpoonup j_r$ in $L^1([0, T])$ and $\rho_i^\varepsilon \rightharpoonup \rho_i$. For the limit $\sigma \rightarrow 0$, we simply observe that $\rho_i + \sigma \geq \rho_i$ which implies that $\frac{|f_i|^2}{\rho_i + \sigma} \leq \frac{|f_i|^2}{\rho_i}$. Moreover, we have $\nabla \sqrt{\rho_i + \sigma} = \frac{\sqrt{\rho_i}}{\sqrt{\rho_i + \sigma}} \nabla \sqrt{\rho_i} \leq \nabla \sqrt{\rho}$. This proves the desired estimate for the diffusive terms, both the slope and the rate term.

3b (Reactive rate term): The limit $\varepsilon \rightarrow 0$ was shown in Proposition 6.3, where we now rely on Assumption (4.A2) with $p = p_{\text{crit}}$. For the limit $\sigma \rightarrow 0$, we again use the monotonicity of the perspective function, to get the pointwise bound in the integrand

$$\mathbb{C} \left(j_r \left| \sqrt{(\rho_i + \sigma)^\alpha (\rho + \sigma)_i^\beta} \right. \right) \leq \mathbb{C} \left(j_r \left| \sqrt{\rho_i^\alpha \rho_i^\beta} \right. \right).$$

3c (Reactive slope term): We use the general fact that a continuous function $\Phi : \mathbb{R}^f \rightarrow \mathbb{R}$ satisfying the growth estimate $|\Phi(u)| \leq C(1+|u|)^r$ defines via $u \mapsto \Phi \circ u$ a (strongly) continuous Nemitskii operator from $L^{r^q}(\Omega)$ into $L^q(\Omega)$ for all $q \geq 1$.

The reactive slope is the sum $\mathcal{S}_{\text{react}} = \sum_{r \in R} \mathcal{S}_r$ with

$$\mathcal{S}_r(\rho) = 2\kappa_r \iint_{\Omega_T} \left(\omega^{(\beta^r - \alpha^r)/2} \rho^{\alpha^r} - 2\rho^{(\alpha^r + \beta^r)/2} + \omega^{(\alpha^r - \beta^r)/2} \rho^{\beta^r} \right) dx dt =: \mathcal{S}_r^1(\rho) + \mathcal{S}_r^2(\rho) + \mathcal{S}_r^3(\rho).$$

By Assumption 4.A2 all three terms define strongly continuous mappings from $L^{p_{\text{crit}}}$ into L^1 , which implies that $\mathcal{S}_{\text{react}} = \sum_{r \in R} \mathcal{S}_r$ is strongly continuous from $L^{p_{\text{crit}}}$ into $[0, \infty)$. Thus, using $\rho^{\varepsilon, \sigma} \rightarrow \rho$ in $L^{p_{\text{crit}}}$ we can pass to the limit $\varepsilon, \sigma \rightarrow 0$, and the result follows. \square

It remains to prove Proposition 3.14, relating the notions of continuum EDB solutions and weak solutions with each other.

Proof of Proposition 3.14. Under the condition $\rho_i \in [\sigma, 1/\sigma]$ it is standard to show that weak solutions are continuum EDB solutions. Indeed, for $i \in I$, we start from the definition of weak solutions with $\varphi \in L^2(0, T; H^1(X))$ in the form

$$0 = \int_0^T \langle \partial_t \rho_i, \varphi \rangle dt + \int_{\Omega_T} \delta_i \rho_i \nabla \log \left(\frac{\rho_i}{\omega_i} \right) \cdot \nabla \varphi + \sum_{r \in R} \gamma_i^r \kappa_r \omega^{(\alpha^r + \beta^r)/2} \left(\frac{\rho^{\alpha^r}}{\omega^{\alpha^r}} - \frac{\rho^{\beta^r}}{\omega^{\beta^r}} \right) \varphi dx dt.$$

Using $\rho_i \in [\sigma, 1/\sigma]$ we are allowed to choose the test function $\varphi(t) = \log(\rho_i/\omega_i)$ for $t \in [t_1, t_2]$ and 0 otherwise.

Summing over $i \in I$ and using the classical chain rule for \mathcal{E} (now evaluated only on the interval $[\sigma/\omega^*, 1/(\omega_*\sigma)] \subset (0, \infty)$), we obtain

$$\mathcal{E}(\rho(t_1)) - \mathcal{E}(\rho(t_2)) + \int_{t_1}^{t_2} \int_{\mathbb{T}^d} \mathbb{G} D\mathcal{E}(\rho) \bullet (f, j) dx dt = 0$$

where $f = (f_i)_i$ and $j = (j_r)_r$ are given as in (3.9). By the definitions of \mathcal{S} and \mathcal{R} in the Definitions 3.9 and 3.10 with $\mathcal{S}(\rho) = \mathcal{R}^*(\rho, -\mathbb{G} D\mathcal{E}(\rho))$ (as $\rho_i \geq \sigma$), we have the identity $\mathbb{G} D\mathcal{E}(\rho) \bullet (f, j) = \mathcal{R}(\rho, f, j) + \mathcal{S}(\rho)$, which implies that (ρ, f, j) is a continuum EDB solution.

For the opposite direction, we start from a continuum EDB solution (ρ, f, j) such that we have $(\rho, f, j) \in \text{CE}$, and $\mathcal{D}(\rho, f, j) < \infty$, which, under the assumption $\rho_i \in [\sigma, 1/\sigma]$, imply the regularity

$$\rho \in L^2(0, T; H^1(\mathbb{T}^d)), \quad f \in L^2(\Omega_T), \quad j \in L^1(\Omega_T), \quad \partial_t \rho \in L^2(0, T; H^{-1}(\mathbb{T}^d)) + L^1(\Omega_T).$$

Moreover, the derivative $D\mathcal{E}(\rho) = (\log(\rho_i/\omega_i))_{i \in I}$ is well-defined in $L^2(0, T; H^1(\mathbb{T}^d))$ and satisfies the identity $\mathcal{S}(\rho) = \mathcal{R}^*(\rho, -\mathbb{G} D\mathcal{E}(\rho))$. Together, this is enough to establish the chain rule

$$\begin{aligned} \frac{d}{dt} \mathcal{E}(\rho(t)) &= \langle \partial_t \rho, D\mathcal{E}(\rho) \rangle = \langle \mathbb{G} D\mathcal{E}(\rho), (f, j) \rangle \\ &= \int_{\mathbb{T}^d} \sum_{i \in I} \nabla \log \left(\frac{\rho_i}{\omega_i} \right) \cdot f_i + \log \left(\frac{\rho}{\omega} \right) \bullet \Gamma^* j dx. \end{aligned}$$

Inserting this into the relation $\mathcal{L}(\rho, f, j) = 0$ for continuum EDB solutions and using that $\mathcal{S}(\rho) = \mathcal{R}^*(\rho, -\mathbb{G} D\mathcal{E}(\rho))$, we obtain

$$\langle \mathbb{G} D\mathcal{E}(\rho), (f, j) \rangle = \mathcal{R}(\rho, f, j) + \mathcal{R}^*(\rho, -\mathbb{G} D\mathcal{E}(\rho)) \quad \text{for a.a. } t \in [0, T].$$

Since $\rho_i \geq \sigma > 0$, we conclude $(f, j) = D_{(\xi, \zeta)} \mathcal{R}^*(\rho, -\mathbb{G} D\mathcal{E}(\rho))$ which provides the desired flux relations (3.9) a.e. in $[0, T] \times \mathbb{T}^d$. The fact that ρ is a weak solution follows now from the fact that (ρ, f, j) satisfies the continuity equation CE in the sense of distributions, i.e., $\partial_t \rho = \mathbb{G}^*(f, j)$. \square

A Proof of the magical estimate (3.4d)

Throughout, we consider $p > 1$. With $\lambda_B(r) = r \log r - r + 1$ and $U_p(w) = \frac{1}{p(p-1)}(w^p - pw + p - 1)$ we have the identity

$$w \lambda_B \left(\frac{c}{w} \right) = \frac{p-1}{p} \lambda_B(c) - (p-1)U_p(w) + \frac{1}{p} w^p \lambda_B \left(\frac{c}{w^p} \right) \geq \frac{p-1}{p} \lambda_B(c) - (p-1)U_p(w), \quad (\text{A.1})$$

see [FH*22, Eqn. (2.7)] for an earlier occurrence. Our function C is the convex conjugate of C^* , which is the sum of two exponentials. Hence, C can be written as an infimal convolution, namely

$$C(s) = \min \{2\lambda_B(a_1) + 2\lambda_B(-a_2) \mid a_1 + a_2 = s\}. \quad (\text{A.2})$$

Combining this representation with (A.1) we obtain a lower estimate on $\mathbb{C}(a|w) = wC(a/w)$ that corresponds to (A.1).

Proposition A.1 (Magical estimate for \mathbb{C}). *For all $s \in \mathbb{R}$, $w > 0$, and $p > 1$ we have*

$$\mathbb{C}(s|w) \geq \begin{cases} C(s) & \text{for } w \in [0, 1], \\ \frac{p-1}{p} C(s) - 4(p-1)U_p(w) & \text{for } w \geq 1. \end{cases}$$

Proof. The estimate for $w \in [0, 1]$ follows directly from the monotonicity (3.4b).

For $w \geq 1$ we exploit the infimal convolution (A.2) and (A.1) to obtain the following chain of estimates:

$$\begin{aligned} \mathbb{C}(s|w) &\stackrel{(\text{A.2})}{=} 2 \min_{a_1+a_2=s} \{w\lambda_B(a_1/w) + w\lambda_B(-a_2/w)\} \\ &\geq 2 \min_{a_1+a_2=s} \left\{ \frac{p-1}{p} \lambda_B(a_1) - (p-1)U_p(w) + \frac{p-1}{p} \lambda_B(-a_2) - (p-1)U_p(w) \right\} \\ &\stackrel{(\text{A.2})}{=} \frac{p-1}{p} C(s) - 4(p-1)U_p(w). \end{aligned}$$

This is the desired estimate for $w \geq 1$. □

The desired magical estimate (3.4d) now follows from $U_p(w) \leq w^p/(p(p-1))$ for $w \geq 1$ and Proposition A.1 by rearranging the estimate.

The main usage of the estimate is in the integrated form namely

$$\int_{\Omega} C(s) \, d\mu \leq \frac{p}{p-1} \int_{\Omega} \mathbb{C}(s|w) \, d\mu + \frac{4}{p-1} \int_{\Omega} w^p \, d\mu.$$

The following example shows that estimating the integral on the left-hand side by the two integrals on the right-hand side is not possible for the case $p = 1$, i.e. $p > 1$ is essential. We give an example with $\int_{\Omega} \mathbb{C}(s|w) \, d\mu + \int_{\Omega} \lambda_B(w) \, d\mu < \infty$ but $\int_{\Omega} C(s) \, d\mu = \infty$.

Remark A.2 (Counterexample). *We let $\Omega =]0, 1/2[$, take $\mu = L^1$ and choose*

$$s(x) = \frac{1}{x(\log(1/x))^\gamma} \quad \text{and} \quad w(x) = \frac{1}{x(\log(1/x))^\omega} \quad \text{with } 1 < \gamma < 2 < \omega.$$

This gives $s \in L^1(\Omega)$, $\int_{\Omega} \lambda_B(w) \, dx < \infty$, and $\int_{\Omega} C(s) \, dx = \infty$. With $s(x)/w(x) = (\log(1/x))^{\omega-\gamma}$ and $C(r) \approx r \log(1+r)$ for $r \gg 1$ we find $\int_{\Omega} \mathbb{C}(s|w) \, dx < \infty$.

B Superlinear functions: Proof of Lemma 3.3

Lemma 3.3 involves the superlinear functions ϕ and ψ and constructs another superlinear function $\Xi = \Xi_{\phi, \psi}$. It is a generalization of (3.4d) which corresponds to $\phi = C$ and $\psi(w) = cw^p$ with $p > 1$. Then ψ_C can be estimated below by $c_p C$.

It is easy to see that Ξ is even and increasing on $[0, \infty)$ as $s \mapsto w\phi(s/w)$ is so for each $w > 0$. As ψ is increasing and $w \mapsto w\phi(s/w)$ is decreasing (as $s\phi'(s) \geq \phi(s)$) we have the lower estimate

$$\Xi(s) \geq \min\{w_*\phi(s/w_*), \psi(w_*)\} \quad \text{for all } w_* > 0,$$

and it remains to choose w_* appropriate for each s .

The superlinearity of ψ provides for each $M > 1$ a $w_M \geq 1$ such that $\psi(w_M) \geq Mw_M$. For $s_M = M^{1/2}w_M$ and using $\mathbb{C}(s|w) = wC(s/w)$ we thus obtain

$$\frac{\Xi(s_M)}{s_M} \geq \min \left\{ \frac{w_M\phi(s_M/w_M)}{s_M}, \frac{\psi(w_M)}{s_M} \right\} = \min \left\{ \frac{\phi(M^{1/2})}{M^{1/2}}, M^{1/2} \right\} \rightarrow \infty$$

for $M \rightarrow \infty$, which implies $s_M \rightarrow \infty$. As Ξ is increasing on $[0, \infty)$, the desired superlinearity of Ξ and Lemma 3.3 are established.

C Gagliardo-Nirenberg

To prove Proposition 5.4, we will use a variant of the Gagliardo-Nirenberg estimate handling spatial and temporal integrability according to the a priori estimates from the L^∞ bound for the energy and the L^2 bound for the dissipation. We will use the classical dimension-dependent Gagliardo-Nirenberg estimate

$$\|u\|_{L^q(\mathbb{T}^d)} \leq C_{q,d} \|u\|_{L^2(\mathbb{T}^d)}^{1-\theta_q} \|u\|_{H^1(\mathbb{T}^d)}^{\theta_q} \quad \text{with } \theta_q = \frac{d}{2} - \frac{d}{q},$$

where $q \in [2, \infty)$ and $(d-2)q \leq 2d$. With this, we obtain for $\alpha > 0$ and $r \geq 1$ with $\alpha r \geq 2$ and $(d-2)\alpha r \leq 2d$ the estimate

$$\begin{aligned} \iint_{\Omega_T} u^\alpha v \, dx \, dt &\leq \int_0^T \|u(t)\|_{L^{\alpha r}(\mathbb{T}^d)}^\alpha \|v(t)\|_{L^{r'}(\mathbb{T}^d)} \, dt \\ &\leq C_{\alpha r, d}^\alpha \|v\|_{L^\infty([0, T]; L^{r'}(\mathbb{T}^d))} \|u\|_{L^\infty([0, T]; L^2(\mathbb{T}^d))}^{\alpha(1-\theta_{\alpha r})} \int_0^T \|u(t)\|_{H^1(\mathbb{T}^d)}^{\alpha\theta_{\alpha r}} \, dt, \end{aligned} \tag{C.1}$$

where $r' = r/(r-1)$ is the dual exponent of r .

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